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Practical Demonstration of Urban Air Quality Simulation Models. Part I: A Report of the NATO/CCMS Pilot Study on Air Pollution Assessment Methodology and Modeling

NATO Committee on the Challenges of Modern Society, Brussels (Belgium)

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THE CHALLENGES OF
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Number 106

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16. ABSTRACT

This document is the pilot study working towards a standardization of Gaussian plume models for specific air quality management applications. It summarizes the essential elements required of a Gaussian Plume model, compares the models participating in the Practical Demonstration, and compiles and evaluates the results of this model. It contains the full length papers prepared for the Practical Demonstration. These discuss: The "Common Data Base" used for the Test City, brief descriptions of the models used in the Practical Demonstration, and the results of the model calculations for the Test City.

Contains bibliography, list of participants in the Practical Demonstration, and list of panel members with their addresses, and a list of all NATO/CCMS Documents on the First Air Pollution Pilot Study.

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Practical Demonstration of Urban Air Quality Simulation Models
- Part I -

A Report of the NATO/CCMS Pilot Study on Air Pollution Assessment Methodology and Modeling

COMMITTEE ON THE CHALLENGES OF MODERN SOCIETY
NORTH ATLANTIC TREATY ORGANIZATION
(August 1980)

Preface

The North Atlantic Treaty Organization (NATO) established the "Committee on the Challenges of Modern Society" (CCMS) at the November 1969 meeting of the North Atlantic Council.

The CCMS was charged with developing meaningful environmental and social programs that complement other international programs, and with showing leadership, first, in solution of existing problems and, second, in development of long-range goals for environmental protection in the NATO sphere of influence and in other countries as well. A first Pilot Study on Air Pollution was initiated by the CCMS at its inaugural meeting in December 1969. The United States (Environmental Protection Agency) has been the pilot nation with the Federal Republic of Germany (Federal Ministry of the Interior) and Turkey (Scientific and Technical Research Council) as copilot-nations.

The Pilot Study on Air Pollution was an action program designed to demonstrate and encourage the utilization of existing knowledge for the development of air quality management programs. It entailed the demonstration of a system approach to air quality management. Case studies have been carried out in Ankara, Turkey; Frankfurt, Federal Republic of Germany; St. Louis, U. S.; Oslo, Norway; South Holland Region, The Netherlands (NATO/CCMS Report No. 6, Appendices A - E).

The results of the pilot study are documented in NATO/CCMS Report No. 6 (Revised) "Guidelines to Assessment of Air Quality" of October 1972 and in NATO/CCMS Report No. 33 (Final Report) containing 15 recommendations as well as in several other documents, listed as Annex II to this document.

Starting from three of the above recommendations (VI, VII and XIV) the Federal Republic of Germany proposed to initiate a new Pilot Study on Air Pollution Assessment Methodology and Modeling at the CCMS Plenary Session on October 22 and 23, 1974.

These NATO/CCMS Recommendations are:

RECOMMENDATION VI

Member nations will co-operate to develop standardized methods for emissions data storage and retrieval to support requirements in the conduct of national air quality management programs. The US National Emission Data System (NEDS) might serve as a model for a common international system.

RECOMMENDATION VII

Member nations will co-operate to develop standardized techniques for projecting emissions and predicting future ambient air quality.

RECOMMENDATION XIV

Member nations agree the CCMS modeling activity has shown that there is a widespread need for further international co-operation to accomplish the following tasks:

Bring together model developers and air quality managers for exchange of ideas, discussion of users' needs and demonstration of modeling techniques.

Standardize modeling techniques for specific air quality management applications and consider how computerized models might be made available for all users.

Continue to review on-going air quality assessment studies.

In spring 1975 the North Atlantic Council approved the German proposal. The pilot study work started with the Federal Republic of Germany (Federal Ministry of the Interior) as pilot nation and the United States of America (Environmental Protection Agency) and Belgium (Service du Premier Ministre) as co-pilot nations:
A Working Group and two Panels were established with the following functions:

Assessment Methodology Panel

- Pursue and carry out Recommendations VI and VII
- Continue to review present and future assessment studies with respect to the application of assessment methodology.

Modeling Panel

- Develop standardized models for various air quality management applications.
- Develop programs to improve modeler/user communications in conjunction with the Assessment Methodology Panel and the Working Group.
- Continue as an information forum on new modeling concepts and techniques, organizing once a year international technical meetings on air pollution modleing and its application.

In addition the Working Group established an Ad-Hoc Group on Air Quality Management Systems to revise and update the NATO/CCMS Report No. 6 (Revised) 1972 by preparing a new document on "Guidelines to Air Quality Management Systems".

Another Ad-Hoc Group was set up for compiling a Glossary of Terms frequently used in assessment methodology, modeling and air quality management systems.

As an outcome of this Pilot Study on Air Pollution Assessment Methodology and Modeling the following NATO/CCMS documents are published (see also Annex III):

Air Quality Management System

- Guidelines to Air Quality Management System.

Assessment Methodology

- Air Pollution Emission Inventory Systems
- Air Pollution Emissions Projecting

Air Pollution Modeling

- Introduction to Air Quality Modeling
- Uses and Needs for Air Quality Modeling
- Bibliography on Grey Literature on Air Quality Modeling, Part I (Applied Models)
- Bibliography on Grey Literature on Air Quality Modeling, Part II (New Modeling Techniques)
- Practical Demonstration of Multiple Source Urban Air Quality Modeling (Gaussian Plume)
- Fundamentals for the Applications of a Gaussian Plume Model

Other Publications

- Glossary of Terms
- Proceedings of the 6th to 9th International Technical Meetings on Air Pollution Modeling and its Application
  (6th Meeting, 24. - 26. Sept. 1975, Frankfurt/Main, Germany)
  (7th Meeting, 7. - 10. Sept. 1976, Airlie House, USA)
  (8th Meeting, 20. - 23. Sept. 1977, Louvain-la-Neuve, Belgium)
  (9th Meeting, 29. - 31. Aug. 1978, Toronto, Canada).

The chairman of the Working Group wishes to acknowledge the scientists participating from pilot, copilot, and observer countries, and the many other persons, who assisted in the preparation of this document.

The panel, which performed diligently throughout the course of this effort, receives the highest praise. The panel members were:

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The addresses of the panel members are listed in Annex I.

Full recognition is given to each panel member for carrying out and coordinating review and other activities related to the development of this document in his respective country and to Ms. C. Morawa of the Federal Environmental Office, Germany for her effort in coordinating and organising and for editorial work.

For the Working Group,
Erich Weber, Chairman.

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Appendix I: List of Participants in the Practical Demonstration of Urban Air Quality Simulation Models

Appendix II: Continuously Measured Concentration Data for Selected Receptor Sites

Annex I: Names and Adresses of Panel Members

Annex II: NATO/CCMS Documents on the First Air Pollution Pilot Study

Annex III: NATO/CCMS Documents on the Pilot Study on Air Pollution Assessment Methodology and Modeling

1. Introduction

A comprehensive survey of models is presented in the NATO/CCMS documentation "Introduction to Air Quality Modeling". Information on the capabilities, applicability and limitations of a special deterministic model to calculate air quality, the Gaussian plume model, is given in the NATO/CCMS document "Fundamentals for the Application of a Gaussian Plume Model". A review of the variety of applications of Gaussian plume models is outlined in the NATO/CCMS document "Uses and Needs of Air Quality Models".

Within this pilot study nearly all tasks listed in Recommendation XIV as given in the preface have been discussed in the NATO/CCMS documents cited above, but one question has still left been open

- standardize modeling techniques for specific air quality management applications.

The term "standardization" has not yet been defined precisely, but a scientific sound standardization of Gaussian plume models should at least reflect the following aspects:

- World-wide registration and examination of the variety of applied and validated Gaussian plume models.

- Investigation of their model structure and parameters, and of the input data to be used.

- Comparative model calculations of Gaussian plume models using an identical set of input data and prescribed model output.

- Evaluation of sensitivity analyses of all these models.

- Clarification and determination of those output data which can be predicted by a standardized Gaussian plume model with sufficient accuracy.

- Determination of the limitations of Gaussian plume models with respect to the given specific air quality management application.

It would be an effort going much beyond the possibilities of just one Pilot Study to investigate all these points and to come to a general, scientific sound "standardization" of Gaussian plume models for specific air quality management applications.

The NATO/CCMS activity "Practical Demonstration of Urban Air Quality Simulation Models", which is summarized in this NATO/CCMS document can, therefore, only be interpreted as a first, but necessary step into this direction of model standardization.

Based on a registration and examination of well known Gaussian plume models being in widespread operational use and an investigation of their main differences, comparative model calculations for a "Test-City" have been performed using a given "Common Data Base". It was the intention to get a first feeling for the possible band width of model output data with res-

pect to the given specific air quality management application, being urban air quality simulation of a multiple source system in this case. Furthermore, such a procedure represents a way in the direction of quantitatively comprehending the limitations of Gaussian plume models, and, thus, may quantitatively show up those regimes where the necessity of applying new modeling techniques can no longer be denied.

The NATO/CCMS document "Practical Demonstration of Urban Air Quality Simulation Models" consists of two parts

Part I containing in summarizing form

- a list of essential elements and data requirements of a Gaussian plume model,
- a synopsis and a comparison of the models participating in the Practical Demonstration,
- a compilation and an evaluation of the model results.

Part II containing in full length the most important original papers which have been prepared when carrying-out the "Practical Demonstration as there are

- the "Common Data Base" for the Test-City,
- brief descriptions of the models participating in the Practical Demonstration,
- all results of the model calculations for the Test-City.

While Part I addresses to those who want to gain an overview over this Practical Demonstration, Part II addresses to those who want to use the full data set for their own evaluations and interpretations.

2. Basic Equations and Elements of a Gaussian Plume Model

Providing that the following prerequisites are fulfilled:

- the atmosphere shows steady state conditions and is homogeneous

- the emissions are constant in respect of quantity and emission conditions throughout the period on which calculations are based (e. g. 1/2 or 1 hour); for shorter-term emissions, the proposed computing methods must be modified,

- the air pollutants (SO_2) are considered in the calculations to be inert nonreactive gases,

- the emitted components undergo no physical or chemical changes during the dispersion process,

- the diffusion area is flat; and dispersion is not decisively disturbed by large buildings or vegetation beyond those turbulent disturbances resulting from a mean surface friction of the diffusion area as included in the diffusion parameters,

- there are no meteorological situations characterized by a reduction in the transport and exchange processes (i. e. calms and light-wind situations with a mean wind speed of less than about 1 or 1,5 m/s at anemometer level).

The spatial concentration distribution of an air pollutant being emitted continuously from a single source may be described by a bivariate Gaussian concentration distribution. For further details, see NATO/CCMS document "Fundamentals for the Application of a Gaussian Plume Model".

Under the assumptions above the bivariate Gaussian distributions reads

a) without an upper inversion (no adsorption at ground)

$$c\,(x,y,z) = \frac{Q}{2\pi u\,\sigma_y\,\sigma_z}\,\exp\left(-\frac{y^2}{2\,\sigma_y^2}\right)$$

$$\left\{\exp\left(-\frac{(z-h)^2}{2\,\sigma_z^2}\right) + \exp\left(-\frac{(z+h)^2}{2\,\sigma_z^2}\right)\right\}$$

b) with an upper inversion at an altitude of H_I (total reflection at H_I)

$$c\,(x,y,z) = \frac{Q}{2\,H_I\,u}\,\frac{\exp\left(-\frac{y^2}{2\,\sigma_y^2}\right)}{\sqrt{2\pi}\;\;\sigma_y}\,\mathcal{O}_3\left(\frac{z-h}{2\,H_I}\;;\;\frac{z^2}{2\,H_I^2}\right)$$

$$+\;\mathcal{O}_3\left(\frac{z+h}{2\,H_I}\;;\;\frac{z^2}{2\,H_I^2}\right)$$

with

$$\vartheta_3\ (V;W) = \frac{1}{\sqrt{\pi}\ W} \sum_{n=-\infty}^{+\infty} \exp\ \left(- \frac{(V+n)^2}{W} \right)$$

In the variety of the models participating in the Practical Demonstration both kinds of equations are being used, as can be seen from the model descriptions in Part II of this document.

The meaning of the symbols in the equations is as follows

(x,y,z)	= location of receptor point in rectangular coordinates with the origin at foot of the source
Q	= source emission rate of the air pollutant
$h = H + \Delta h$	= effective source height
H	= physical source height
Δh	= height of plume above the stack (plume rise)
u	= mean wind speed
σ_y, σ_z	= standard deviations of the horizontal and vertical Gaussian distributions ("dispersion parameters")
H_I	= inversion or mixing height, resp.

From these equations the main elements of Gaussian plume models can be derived easily, the knowledge of which is essential for

- compiling a "Common Data Base",

- analysing the descriptions (see Part II of this document) of the models participating in the Practical Demonstration.

One can distinguish between two classes of "model elements"

- data requirements and model assumptions concerning data processing,

- internal model assumptions with regard to plume rise, meteorological structure of the planetary boundary layer, and dispersion processes.

These two classes of model elements may be illustrated by help of some typical, but not comprehensive examples

- model assumptions leading to the derivation of either daily or seasonal variations or temperature dependent variations of space heating emissions from annually averaged emission statements,

- plume rise formulas, assumptions concerning dispersion parameters and corresponding schemes for atmospheric stability classes, presupposition of a vertical wind profile.

The first class of model elements proves to be necessary to describe the model's requirements for input data with respect to model application. With regard to the "Practical Demonstration of Urban Air Quality Simulation Models" this has to be made concrete in the following sense:

Comparative model calculations of Gaussian plume models require an identical set of input data, i. e. a common data base. To formulate criteria for manner, extent and accuracy of the contents of such a common data base, the data requirements of the Gaussian plume models under concern have to be analysed and to be investigated quantitatively.

The second class of elements, i. e. elements concerning the internal structure of a Gaussian plume model, determines, in the case a common data set is given, differences in calculated immission concentrations as there are for example

- position and intensity of annual mean concentration maxima,
- temporal and spatial field structure of ambient air quality,
- upper percentiles of the cumulative frequency distribution of immission concentrations.

As can be seen from the comparison of models participating in the Practical Demonstration, as presented in chapter 5 of Part I or from Part II of this document a comprehensive quantification of model re-

quirements with respect to all these elements is extremely difficult, because data requirements and internal model parameters often differ considerably from one model to another.

As a consequence of the effects upon model results to be expected from both classes of model elements extensive sensitivity analyses with respect to

- errors in input data or sundry procedures in data-processing as well as

- actual and possible differences in internal model assumptions (e. g. plume rise formula or dispersion parameters)

represent an urgent task for future work on immission prognosis by help of model comparison for standardization purposes.

Some of this work has already been done within this NATO/CCMS Pilot Study Air Pollution.

In chapter 3 possible data requirements (first class of model elements) for a Gaussian plume model are briefly repeated in a general form with the intention to derive criteria for structure and extent of a common data basis (chapter 4) for the Practical Demonstration.

Differences in internal model assumptions of the participating models are worked out in chapter 5.

3. Data Requirements for a Gaussian Plume Model

Within this chapter the main data requirements, which in general could be postulated by a Gaussian plume model are briefly outlined.

The common data base for the "Test-City" which has partly been derived from these general requirements, but had to be adopted to the specific conditions and the informations available for the "Test-City" is described in chapter 4.

3.1 Emission Data

Requirements for Emission Data of Point Sources

Gaussian models require the following details of an emissions inventory:

- position of the installation in a rectangular coordinate system by giving values for
  - x-coordinate and
  - y-coordinate

- annual or seasonal emission rate of pollutant in a model depending dimension (e. g. tons/day, kg/h, g/s) or emission rate of stack gas in a model depending dimension (e. g. m^3/h) and concentration of pollutant (in percentage).

  The time period of emissions and the time period the model calculates for must coincide

- stack parameters as
  - height of the stack of the source (topographical height)
  - inner diameter of the stack exit
  - exhaust flow velocity of stack gas (m/s)
  - stack exit gas temperature.

The stack parameters are necessary to calculate the plume rise. If exhaust flow velocity and temperature of the stack gas vary too much, again a mean value has to be calculated.

Requirements for Emission Data of Area Sources

An area source actually represents a collection of many small sources, each of which may emit only small quantities, but because of their great number the collective impact may be significant. Therefore, emission data of area sources should be given as exact as possible (ref. is made to NATO/CCMS doc. No. 102).

Gaussian models require similar parameters for area sources as for point sources.

- position of the area source in a rectangular coordinate system by giving values for
  - x-coordinate and
  - y-coordinate

- extension of the source (e. g. km^2)

- annual or seasonal emission rate (e. g. tons/day, kg/h, g/s)

- mean height of source area.

For most models the extension of the sources may vary from source to source, though some models require a constant area source grid. For simulating European urban air pollution, area sources are usually not larger than 1 km x 1 km.

The annual or seasonal emission rate of a pollutant is equal to the emission rate of the installation running under normal load. However, in many cases there will be large variations in the load and consequently in the emission rate. In these cases, if the model does not have the facility to cope with variable emission rates, the mean value should be used.

As for point sources it is advisable to take also emissions of area sources outside the examination area as input data. A surrounding area with a width of about 5 km should be broad enough. Influences coming from area sources of greater distances may be taken into consideration as a constant background.

Contrary to point sources most of the models do not consider plume rise for area sources in Gaussian models. Normally the exhaust flow velocity as well as the temperature have small values so that this assumption can be used as a first approximation. Some models, however, use more or less empirical assumptions for the plume rise of area sources. For further details, see the papers by Junod, Liechti and Gutsche, Stern in Part II of this document. On the other hand, the emission niveau is not to be neglected so that it is advisable to use area source heights other than zero.

3.2 Meteorological Data

Gaussian plume models usually require at least the following meteorological input data:

- mean wind direction at anemometer level (about 10 m above ground)
- mean wind speed $\bar{u}$ (m/s or knots) at different levels; at least, at around 10 m height above ground
- the atmospheric stability according to classification schemes like those by Turner or Klug/Manier (only these schemes were used within this practical demonstration)
- inversion - or mixing height H_I (m), resp.
- at least, daily mean temperature $\bar{T}$ (°C), for characterizing the source strength of space heating and of point sources, if appropriate

Multi-dimensional frequency distributions of these parameters in suitable class-intervalls of $\bar{T}$, $\bar{u}$, H_I will be needed to calculate long-term concentration values.

In principle, the temporal resolution and the accuracy of meteorological input data entering a dispersion model should correspond to that of the respective concentration values.

3.3 Immission Data

Immission data (ambient air quality data) are usually not input data to air pollution models, as emission and meteorological data are. They are, however, needed for:

- testing the reliability of modeling systems and results (verification)
- calibration of model output.

The results of ambient air quality measurements should derive the same characteristic values as air pollution modeling results.

These characteristic values of ambient air quality ought to be related

- to ambient air quality standards and/or
- to ambient air quality criteria.

Sampling duration, averaging time and sampling frequency are important when evaluating results of atmospheric air quality measurements. For measurements of gaseous air pollutants a sampling duration (section of measurement) of 15 to 60 minutes is usually recommended.

Characteristic values, which can be derived from concentration measurements and which should be compared with the results of dispersion models, are:

- annual arithmetic mean or geometric mean (if the AQS is specified as such),

- cumulative frequency distribution or, at least, some percentiles of the cumulative frequency distribution.

The measurements must characterize the ambient air quality situation at well-defined sites in the field, because dispersion models likewise calculate concentration values to be expected at such receptor sites.

Siting criteria for measuring stations should be

- that concentration values are obtained, which are of relevance for model calculations,

- that locally influenced concentrations are not predominant, as they cannot be predicted by a dispersion model being developed for a non-local, larger scale,

- that the dispersion conditions are not dominated by geographic or topographic features, because common Gaussian plume models may not be applied to such situations.

Nevertheless, the choice of these receptor sites should guarantee a comprehensive test of the model's capability to predict the main properties of the structure of the concentration field, e. g.

- positions of concentration maxima

- gradients within the concentration field,

- orientation of concentration isolines.

Thus, for validation of model calculations and for model calibrations at least three receptor sites should be used. Continuously working monitoring stations should be prefered. They allow a direct comparison of calculated and measured concentration values for an identical set of meteorological situations.

4. Common Data Base

To accomplish a Practical Demonstration of Urban Air Quality Simulation Models (Gaussian Plume) a data base had to be prepared taking into account as construction criteria

- the general data requirements for a Gaussian plume model as formulated in chapter 3,
- the individual requirements of the models participating in the Practical Demonstration (see Part II of this document),
- the specific conditions of the "Test-City",
- the availability of relevant data.

Due to the sometimes considerably controversial "demands" of these four "boundary conditions" it had been an extremely difficult task of matching to prepare something like a "Common Data Base" or a " Standard Data Base" without being of disadvantage to the one or the other model. The reason for this statement is, that often the theoretical capabilities of dispersion models are going far beyond the availability of input data. On the other hand, this scope of model capability going beyond the

availability of emission and meteorological data seems not to be an adequate measure for the advantages in dispersion model development because till now there has not yet been the possibility of direct model comparison (analogous to this Practical Demonstration) and because of lack of suitable immission data for a problem specific model validation.

The consequence seems to be that further developments in this field can only be made by well-tuned cooperation in model-development, data availability, and corresponding sensitivity analyses.

Bearing this in mind, one had to find a fair compromise between the demands of the four "boundary conditions" cited above. The result was a paper (Common Data Base) which had been sent to the participants of the Practical Demonstration as a basis for their calculations and which can be found (except of emission data) in Part II of this document.

The Common Data Base contains

- explanation of TURNER´s stability classification scheme,

- three-dimensional frequency distributions of TURNER-stability-classes, wind speeds, and wind directions,

- explanation of the KLUG-MANIER-stability classification scheme,

- three-dimensional frequency distributions of KLUG/MANIER-stability-classes, wind speeds, and wind directions,

- SO_2-emissions inventory for residential combustion (for unit areas of 500 m x 500 m the average geometrical emission heights and the annually averaged source strengths (kg/h) are given),

- SO_2-emissions inventory for point sources (position, physical stack height, stack diameter, exit gas temperature and

- exit speeds are given as well as SO_2-output (in kg/h) for the whole year and for heating and non-heating period).

Information concerning inversions or mixing heights were not available for the "Test-City". Furthermore, four-dimensional frequency distributions of meteorological parameters including air temperature (either hourly or as a daily mean value) were not available. Such a multi-dimensional frequency distribution would have allowed a better consideration of the temperature dependent SO_2-emittents, especially space heating. Due to this shortcoming of the "Standard Data Base" especially the calculation of upper percentiles in the cumulative frequency distribution and their comparison with measured values has been deteriorated.

As a first step to take the temperature dependency of SO_2-emittents into account, monthly degree-days for the Test-City. The number of degree days per month is evaluated in the following way:

$$G = Z\ (t_i - t_{am})$$

with

G = number of degree days,

Z = number of days per month, where the daily average temperature has been less than + 15 °C (heating days),

t_i = + 20 °C (desired constant room temperature),

t_{am} = mean value of temperature, formed from the daily mean temperatures of all heating days in the month under concern.

For participants with models allowing for an even more comfortable treatment of meteorological data magnetic tapes with original hourly data of a meteorological station in the "Test-City" have been provided.

In this way "boundary condition" No. 2 (consideration of the individual requirements of the models participating in the Practical Demonstration) could be fulfilled in a flexible way, but, as a consequence of such a differentiated basis of input data, one had to put up with a retrenchment in the requirement of an "identical set of input data" and, thus, with restrictions in the comparability of model output, i. e. calculated concentration fields.

Although, there will never be something like a "universal data base" being ideal and optimized for all models (if not the models are identical) and for all kinds of model applications (see NATO/CCMS doc. No. 101 "Uses and Needs of Air Quality Models"), those basic principles discussed above should be considered whenever a common data base has to be prepared. This re-

presents one of the results which could be derived during the preparation of the Practical Demonstration.

5. Examples of Gaussian Plume Models (Models participating in the Practical Demonstration)

As has already been mentioned in chapter 2, at this place the second class of elements of the models, which have participated in the "Practical Demonstration of Urban Air Quality Simulation Models" will be introduced with their main characteristics.

This second class of model elements comprises all factors marking the internal structure of a Gaussian plume model. Such elements are

- classification assumptions for the essential meteorological and source parameters like
  - wind direction,
  - wind speed,
  - atmospheric stability,
  - inversion or mixing height,
  - daily mean temperature, if necessary,
  - separation between point and area sources,
  - mean source heights for area sources in a grid-square,
  - model assumptions, like
  - treatment of the lateral diffusion (e. g. narrow-plume hypothesis),

  - simplified area-source representations by help of box-model-type assumptions, which are implicitly based on a Gaussian distribution (e. g. ATDL-model).

- formulas, implicitly involving physical, chemical, and meteorological processes into the model equations, e. g.

  - plume rise formula,
  - meteorological structure of the domain of dispersion (i. e. assumptions concerning the horizontal and vertical structure of the planetary boundary layer),
  - consideration of simple physical and chemical transformation processes during the transmission process,
  - mechanisms for a rough and lumped consideration and inclusion of phenomena and situations, which are - in a strict sence - outside the intrinsic range of applicability of a Gaussian plume model, e. g. calm wind situations.

- parameter sets for e. g.

  - horizontal and vertical dispersion parameters,
  - exponents in a power law for the vertical wind profile.

Regarding these main characteristics of internal model structure elements, those models participating in the Practical Demonstration have been analysed with respect

to the most important points of view from which is known by sensitivity analyses that they are influencing calculated immission concentrations effectively. The results of this analysis are presented in table 1. With respect to such a compilation the following fundamental statements should be emphasized:

- the specific advantages, but also disadvantages of the individual models have to be seen in respect of the individual fields of application they have been programmed for (normative efforts and legislatively required conclusions differ from country to country and, thus, from model to model),

- this compilation elucidates the broad spectrum of possible combinations of distinct suppositions, formulas, and parameter sets, whereby has to be noticed, that the frequency of appearance in this table of individual assumptions, formulas or parameter sets does not represent a measure for a specific scientificially sound basis,

- a multiple listing of the same sign or name for a special quantity (e. g. BRIGGS' plume rise formula, PASQUILL's stability classes, SINGER and SMITH' dispersion parameters and so on) does not automatically implicate identical versions and formulations because of a variety of subjective, and not always scientificially confirmed modifications of published results. It must also be emphasized that certain models have different options for plume rise formula, turbulent diffusion schemes (stability classes) and the corresponding dispersion parameters.

Model	Calculation performed by	Plume rise equ.	Wind direction classes	Wind speed classes	Vertical wind profile	Stability classes	Dispersion parameters	Inversion, mixing height	Daily mean temperature	Remarks / similar to
KILDER	**SIVERTSEN**	Combination of HOLLAND, BRIGGS, STÜMKE II	12	4	constant with height	4 classes $\frac{\partial \theta}{\partial z}$	MP + SS	input in each class of wind/ stability	-	
FORTAK	STERN GUTSCHE TIMM	1. STÜMKE I+II 2. MOSES & CARSON	36	6	power law	TURNER 5 classes	MP + SS	by choice	6 classes	area sources for $Q \leq 1$ kg/h
KNMI	NIEUWSTADT	BRIGGS	12	3	power law	PASQUILL 6 classes modified	PG + SS + Interpolation	5 classes	-	CDM
TÜV Rheinland	KROPP SCHNEIDER	MOSES & CARSON (neutral)	36	10	power law	1. KLUG/ MANIER 2. TURNER 6 classes	1. POLSTER /VOGT 2. MP+SS	by choice	in form of degree days	
CDM	BATTELLE Germany	BRIGGS	36	6	power law	KLUG	PG (modified by KLUG)	prescribed for each stability class	-	CDM area
ATDL	BATTELLE Germany	BRIGGS	16	6	power law	KLUG	PG (modified by KLUG)	prescribed for each stability class	in form of degree days	sources for $Q \leq 5$ kg/h
TCM	CHRISTIANSEN PORTER	BRIGGS	16	6	power law	TURNER 6 classes	PG	-	-	area sources according to HANNA GIFFORD

Table 1: Main characteristics of Gaussian plume models participating in the practical demonstration of urban air quality simulation models.

MP = McElroy & Pooler, PG = Pasquill & Gifford, SS = Singer & Smith

Model	Calculation performed by	Plume rise equ.	Wind direction classes	Wind speed classes	Vertical wind profile	Stability classes	Dispersion parameters	Inversion, mixing height	Daily mean temperature	Remarks / similar to
TEM	CHRISTIANSEN	BRIGGS (diff. equs)	any wind direction	any wind speed	power law	TURNER 6 classes	PG	-	-	area sources according to HANNA, GIFFORD
LPADM	BERGER et al	BRIGGS	16	6	power law	PASQUILL 6 classes	PG			CDM
IFDM	KRETZSCHMAR et al.	STÜMKE II	16	6	power law	PASQUILL (modified) 5 classes E + F	PG	freely chosen		area sources for Q ≤ 2 kg/h
CDM	TURNER	BRIGGS	1. 16 2. 36	6	power law	PASQUILL (modified) 6 classes	PG modified + initial spread	representative value f. each stability class	-	
SCAM	IRWIN	BRIGGS	36	6	power law	PASQUILL (modified) 6 classes	PG modified	representative value for each stability class	-	
WARREN SPRING LAB.	HEDDIE, WILLIAMS	BRIGGS	12	mean wind speed in sectors	option for 1. const. with height 2. power law	optional	input parameter	-	-	

Model	Calculation performed by	Plume rise equ.	Wind direction classes	Wind speed classes	Vertical wind profile	Stability classes	Dispersion parameters	Inversion, mixing height	Daily mean temperature	Remarks	similar to
POLLUX	JUNOD/ LIECHTI	BRIGGS	any	any	power law	PASQUILL (modified) 4 classes	NP + Swiss Met.Inst. modified SUTTON by choice	freely chosen, input parameter for each episode	no		
ATDL	GIFFORD				power law	PASQUILL	PG	-	-	it has been called for more detailed information	
ATDL	SANTOMAURO et al	no information available	16		power law	PASQUILL	PG	-	-	simplifying assumptions for meteorology	

Here again, no universal prescriptions or recipes for a unique procedure with regard to model standardization do exist; the best elementary way again seems to be a comprehensive sensitivity analysis.

In the following, an overview shall be given concerning some of the differences between distinct Gaussian plume models, largely based upon table 1. For further, more extensive studies the reader is referred to the original papers (brief model descriptions in Part II of this document).

It has to be recognized that within the broad variety of detail questions several have, looked upon them separately, only an effect of just some percent upon the calculated annual mean values of a multiple-source system like an urban area; but taking all these together the total effect may sum up to about 50 or 100 %.

According to the causal chain

EMISSION - TRANSMISSION - IMMISSION

the aim, therefore, is to single out some of the most essential and effective internal model elements to demonstrate existing differences between several Gaussian plume models in operational use and to elucidate these effects by help of an example for a sensitivity analysis for a Gaussian plume model.

On this basis, as the three main kinds of differences between distinct Gaussian plume models should be outlined:

- differences with respect to source properties (type of source and its representation; plume rise formula),

- differences with respect to transmission factors (classification of wind direction and wind speed, inversion height, atmospheric stability and corresponding dispersion parameters, reduction rates due to physical and chemical transformation rates, boundary conditions),

- differences with respect to model output and resulting statements (e. g. annual mean values of ambient air quality, cumulative frequency distribution, other ambient air quality standards).

a) Differences with respect to Source Properties

The main differences between several Gaussian plume models with respect to source properties result from

- the quantitative differentiation between point and area sources,

- the representation of area sources,

- the choice of a suitable plume rise formula.

The differentiation between point and area sources is commonly tied up to the SO_2-source strength: sources with an emission less than a given limiting

value (ranging from 1 kg SO_2/h in Fortak's model (see GUTSCHE, STERN (1977)) to 5 kg SO_2/h in Battelle/Frankfurt's application of the CDM-model (see BRAIG (1975)) being assigned to area sources.

Several plume rise formulas for point sources are used in Gaussian plume models, e. g.

- HOLLAND (by TIKVART and MARTIN, KOOGLER),
- STÜMKE I or II (BOWNE; FORTAK, GUTSCHE and STERN; KRETZSCHMAR et al.),
- TVA (ROBERTS),
- CONCAWE (SHIEH),
- BRIGGS in different versions (CALDER CCDM; NIEUWSTADT; BERGER et al., CHRISTIANSEN and PORTER; IRWIN; KEDDIE and WILLIAMS; JUNOD and LIECHTI),
- MOSES and CARSON (KROPP and SCHNEIDER; STERN, GUTSCHE and TIMM).

An interesting and promising approach is applied in the Norwegian Kilder-model by SCHJOLDAGER and SIVERTSEN using a differentiated scheme of plume rise formulas:

- HOLLAND's formula for stacks with small heat emission and for unstable and neutral atmospheric conditions,

- STÜMKE's formula to those with medium, and the corresponding BRIGGS-formula to those with large heat emissions, for unstable and neutral stratification,

- BRIGGS' stable stratification formula for a stably stratified atmosphere and for all magnitudes of heat emission.

Such a procedure seems to be a step in the right direction though a well-tuned adjustment of different plume rise formulas has still to be achieved.

In a special version of the KNMI-model (see VERMAAS and NIEUWSTADT (1975)) for comparative investigations two versions of BRIGGS' formulas as well as STÜMKE's-, the CONCAWE-, and the KSLA-formula have been studied.

Detailed investigations of the validity of several plume rise formulas (e. g. MOSES and KRAIMER (1972)) demonstrated that the suitable range of applicability of most of these formulas depends upon

- the type of the source (momentum or buyoant plume),

- the magnitude of the heat emission,

- consideration of atmospheric stability.

Thus, a differentiated combination of different plume rise formulas with respect to their corresponding adequate conditions should be a scientificially sound basis for calculating plume rise.

Due to the considerable differences between all these formulas and their range of applicability (MOSES, KRAIMER (1972)); v. FALSER et al. (1972); LEHMANN (1968); GUTSCHE and LENSCHOW (1973)), the choice of suitable plume rise formulas appears to be one of the most important factors in the field of a rational standardization of Gaussian plume models.

As a consequence, the reaction of an immission concentration field on variations of the effective stack height has to be studied. Such sensitivity analyses have been performed and published by GUTSCHE and LENSCHOW (1973); MASSER and HAMMERLE(1975); PORTER and WOLBACH (1975). As an example for the general procedure the sensitivity analysis of the immission concentration field with respect to the effective stack height will be elucidated at this place.

The intention of a sensitivity analysis is

- to ascertain those parameters which mainly affect the model results,

- to estimate the error band width in the calculated concentration values due to uncertainties in these parameters,

- to make out those points of weakness where further studies should be initiated.

A sensitivity analysis can be performed by two slightly different methods (STERN, GUTSCHE, TIMM (1977))

- by analytical investigation of error equations using the formal definition of "Sensitivity" as the partial derivative of the concentration equation with respect to parameters and input data (see e. g. PORTER and WOLBACH (1975)),

- by the more experimental way of looking at incremental changes in model output resulting from an incremental changes in input data (see e. g. KOCH and THAYER (1971)).

The second method seems to be more appropriate for such complex problems like multiple-source urban diffusion models.

A combination of both methods has been applied by GUTSCHE and LENSCHOW (1973).

The sensitivity S_h of a Gaussian plume ground-level concentration field c (x,y,0) with respect to variations in the effective stack height h is defined by

$$S_h := \frac{\partial c}{\partial h} = - \frac{h}{\sigma_z^2} c$$

which represents a complicated function of the source distances x and y, of atmospheric stability and surface roughness, and of the effective stack height h itself.

The derivative of S_h with respect to the source distance x for fixed effective stack height h yields with

$$g \left(\frac{h^2}{z^2} - 3\right) - f = 0$$

a condition for the position of maximal sensitivity $S_{h,\,max}$ of the concentration distribution beneath the plume axis.

Here, f and g are the exponents in a power law for the dispersion parameters σ_y and σ_z

$$\sigma_y = F\, x^{f} \quad ; \quad \sigma_z = G\, x^{g} .$$

Under the similarity assumption of disperison in y- and z-direction

$$\frac{1}{\sigma_y} \frac{\partial \sigma_y}{\partial x} = \frac{1}{\sigma_z} \frac{\partial \sigma_z}{\partial x}$$

which is often applied in diffusion theory, we obtain

$$f = g$$

(this assumptions holds especially for near neutral conditions)

and the condition above can be simplified to

$$\sigma_z = \frac{h}{2} \qquad \text{for} \quad x\ (S_{h,\,max}).$$

Under the same assumption the position of maximal ground-level concentration is given by

$$\sigma_z = \frac{h}{\sqrt{2}} \qquad \text{for} \quad x\ (c_{max}).$$

The assessment of calculated concentration values and the requirements concerning the plume rise formula and the accuracy of emission input data should be derived on the basis of these results.

The differences between participating Gaussian plume models with respect to area sources can be summarized in two aspects

- area source representation and
- area source plume rise.

Area sources are simulated commonly by use of

- virtual point sources (e. g. TIKVART and MARTIN; KOOGLER; SCHJOLDAGER and SIVERTSEN),
- line sources (GIFFORD and HANNA; SANTOMAURO et al.; CHRISTIANSEN and PORTER, JUNOD and LIECHTI),
- point sources, equally distributed over the grid square (FORTAK, GUTSCHE, and STERN; CALDER (CDM); BRINGFELT et al.).

- circular areas of constant emission density (KRETZSCHMAR et al.)

For area sources plume rise is usually not taken into account in most of the dispersion models; in these cases the mean building height of a grid-square is interpreted as effective emission height. If the separation value between point- and area-sources is given by SO_2-emissions as high as 5 kg SO_2/h this seems to be a quite crude approximation.

Therefore, in FORTAK's model as well as in the POLLUX-model (JUNOD and LIECHTI) semi-empirical assumptions for area source plume rise have been used.

b) Differences with respect to Meteorological Parameters

Though the three-dimensional field of meteorological variables influencing the transmission process over urban areas is generally quite complex, in Gaussian models this description is commonly reduced to a set of very few input data which are supposed to be representative for a large, but homogeneous area. Such parameters are

- wind direction at anemometer level,

- wind speed at anemometer level and assumptions concerning the vertical wind profile,

- atmospheric stability and the corresponding dispersion parameters,

- inversion height or mixing depth,

- daily mean temperature determining the emission of space heating.

To obey the assumption of steadiness, which is inherent in Gaussian plume models, hourly or three-hourly values of these parameters are taken. Weak-wind situations and accumulation periods are excluded in Gaussian plume models, which, however, is not valid for integrated Gaussian puff models if the required parameters are known.

For practical reasons the values of the parameters above are assigned to class intervals, and from their multi-dimensional frequency distribution the dispersion climatology for the region under concern may be derived. This is a necessary presupposition for long-term prediction of the ambient air quality situation.

With respect to the list of parameters above and their classification there exist considerable differences in the dispersion models which are in operational use in many countries. The main differences are listed in the following table.

Furthermore, nearly each dispersion model has its own model-specific modification of intrinsic functions and parameters. Therefore, attention shall be drawn to very few points only

- obviously, the temperature-dependent variation of the SO_2-emission of space heating with the help of daily mean temperature has been considered only in few models,

- the use of inversion height statistics for long-term predictions should be improved,

- there are large differences in the number of wind speed- and wind direction classes, which will be of importance for regions with pronounced maxima of the wind rose (e. g. Frankfurt/M., Germany, for which the first "Practical Demonstration" shall be performed), consequences of such a grouping have partly been studied by BRINGFELT et al. (1974),

- the use of many different sets of dispersion parameters and their individual modification reflects the missing knowledges about the turbulence structure of the mixing layer under arbitrary meteorological and topographic conditions,

- the problem of assigning dispersion parameters derived for a special stability classification scheme to another scheme (e. g. SINGER and SMITH' values to TURNER-classes) has not yet been clarified in a satisfying way.

Concerning the last two points data analysis of tracer experiments like those by BULTYNCK, MALET (1969, 1972); VOGT, GEISS (1974); MÜLLER (1975); and comparative studies like those by KLUG (1969); MANIER (1975); DILGER, NESTER (1975); NIEUWSTADT (1975); SCHULTZ, VOELZ (1975) have to be connected with a comprehensive sensitivity analysis, first steps in this direction are the papers by THAYER, KOCH (1972); GUTSCHE, LENSCHOW (1973); STROTT, CHRIST (1975); KRETSCHMAR ET AL (1978)

c) Differences with respect to Model Output

There exist two kinds of output conceptions for dispersion models

- source-oriented models,
- receptor-oriented models.

Source-oriented models commonly predict concentration fields for an equally spaced grid.

For practical reasons it is often advisable to use a receptor-oriented dispersion model which allows to calculate concentrations for few arbitrarly placed receptor sites. Such a procedure permits a direct comparison between measured and calculated values at a minimum of computation time. The "Practical Demonstration" of air quality dispersion models should reflect both points of view

- representation of the entire field structure,

- direct model validation making use of available measuring series from existing measuring stations.

Long-term model calculations usually result in some of the following specifications

- annual mean values (arithmetic and/or geometric),
- cumulative frequency distributions,
- particularly defined ambient air quality standards (ref. is also made to NATO/CCMS doc. No. 71 rev.),
- time series of subsequent stationary meteorological situations (only as a first approximation because statistical assumptions are inherent in the concept of a Gaussian plume model) (see e. g. KRETZSCHMAR et al. (1978 a).

Comparative model investigations (FORTAK, GUTSCHE, STERN (1975), BRAIG (1975)) show that, in spite of several differences in the calculated annual mean concentration fields, this annual mean value does not seem to be a sensitive instrument for model verifications, cumulative frequency distributions appear to be a more appropriate, more sensitive instrument. Concerning other more sophisticated validation techniques, reference is made to GRØNSKEI (1975).

6. Compilation and evaluation of model results

It has to be recognized that most of the models which have participated in the "Practical Demonstration of Urban Air Quality Simulation Models" were not specifically developed for the necessities of comparative model calculations, but mainly in view of taking into account criteria in urban air quality modeling country-specific for e.g.

- cause analysis
- licensing procedures (determination of the ambient air quality at present in connection with parallel concentration measurements) and
- for the development of control strategies, e. g. for clean air plans or for urban and regional planning activities.

Within the limits of the Gaussian plume assumption the following problematic points may have to be considered by the evaluation of different models, e.g.

- structure and code form of available emission data (see for instance the NATO/CCMS documents of the Assessment and Methodology Panel)
- quality and structure of available meteorological model input data
- that the conception is adapted too much to country-specificly differing ambient air quality criteria
- correction factors for calms, weak-wind situations, local circulation systems, topography, surface roughness and so on

- consideration of background concentrations (see for instance HANNA and GIFFORD'S concept)
- availability of immission concentration data for model validation or calibration.

Due to such different starting positions the respective special problems require that not only just one Gaussian plume model (in the frame of its capabilities) may be considered as optimal. Thus, model structure, model parameters, and input data should have to be adapted to the specific individual aspects cited above. Due to this cause - besides others, which still have to be discussed - it cannot be expected to derive "recommendations" or a world-wide standardization of Gaussian plume models from the results of this "Practical Demonstration".

6.1 Main Differences between Model Results

The model output shall represent an appropriate measure for an assessment of ambient air quality, i.e. it shall demonstrate the model's capability to predict first of all - as mentioned already in chapter 3.3 - the annual mean properties of the structure of the urban ground-level concentration field, e. g.

- positions of concentration maxima
- gradients within the concentration field
- orientation of concentration isolines.

Much more difficult is it to predict other air quality criteria, e. g. cumulative frequency distributions. Comparative model calculation shall therefore help to gain a feeling

- for the reliability of model calculations, when they are compared with measured data,
- for the band with of model calculations, and
- for the ability of models to resolve certain field structures, and aspect, which is of importance for representivity analyses of measuring sites with regard to data assessment.

Due to the rarely available continuously working monitoring networks giving homogeneously distributed values for the whole area under concern - the "Test-City" for the "Practical Demonstration" does not belong to these - at this place first of all a cross-analysis of the results of the different models shall be presented. A comparison with existing measured data will be presented in chapter 7.

The fields of calculated annual mean ground-level concentration values are shown in the following figures 1 to 15.

For selected receptor sites (see table 2) the calculated annual mean ground-level concentration values are being presented (table 3). In the ATDL-model calculations by Gifford the assumed background concentration of about 40 $\mu g/m^3$ has been subtracted to make the model results comparable.

Table 2: Coordinates of Receptor Sites for which Calculations have been performed

No.	GAUSS-KRÜGER		"Test-City"	
1	347329	555153	2229	2653
2	347925	555315	2825	2815
3	347576	555398	2476	2998
4	346700	555200	1600	2700
5	347000	555700	1900	3200
6	348500	555200	3400	2700

Übersichtskarte von Frankfurt/M. und Umgebung

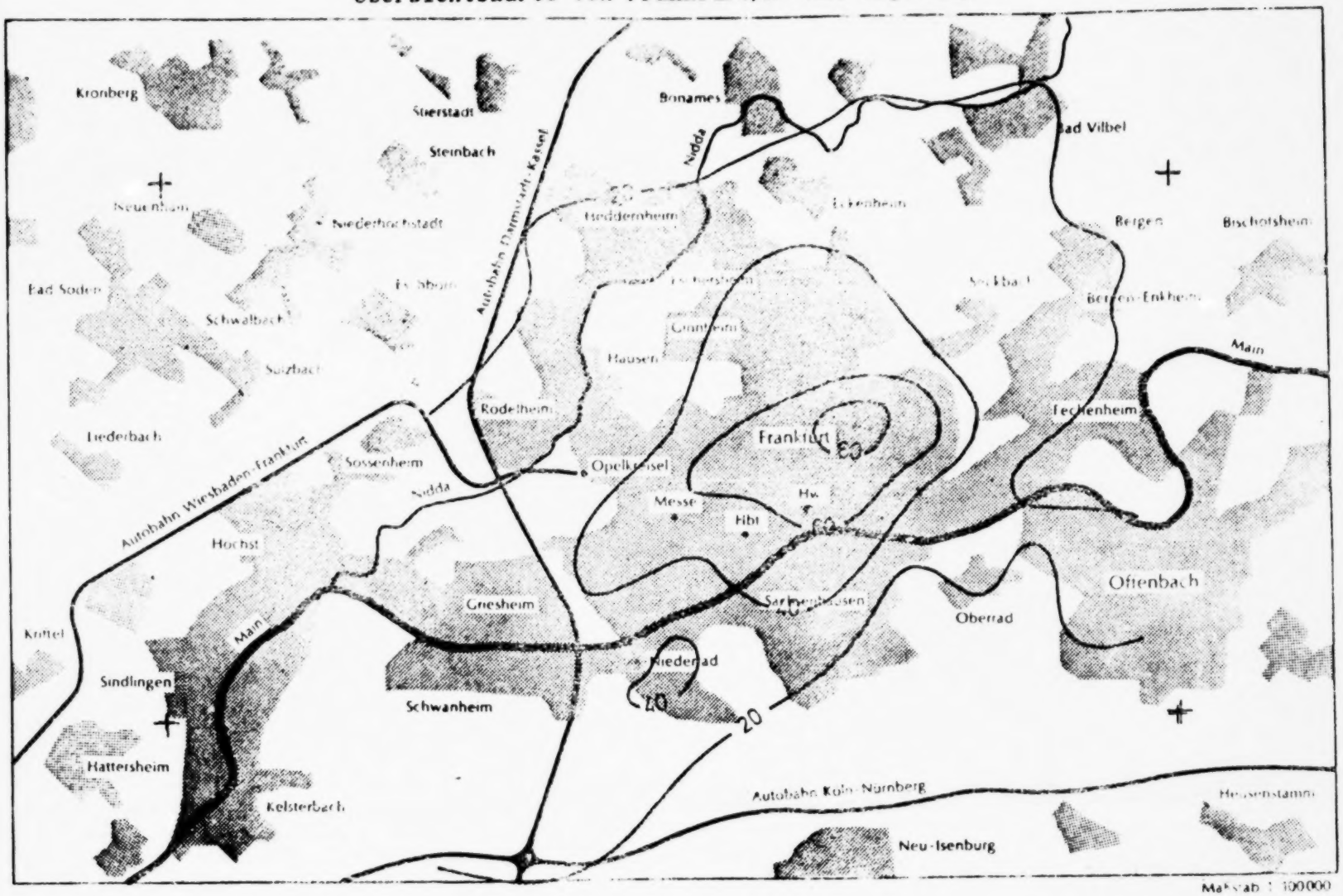

Figure 1 Model: KILDER

Calc. by: Schjoldager, Sivertsen

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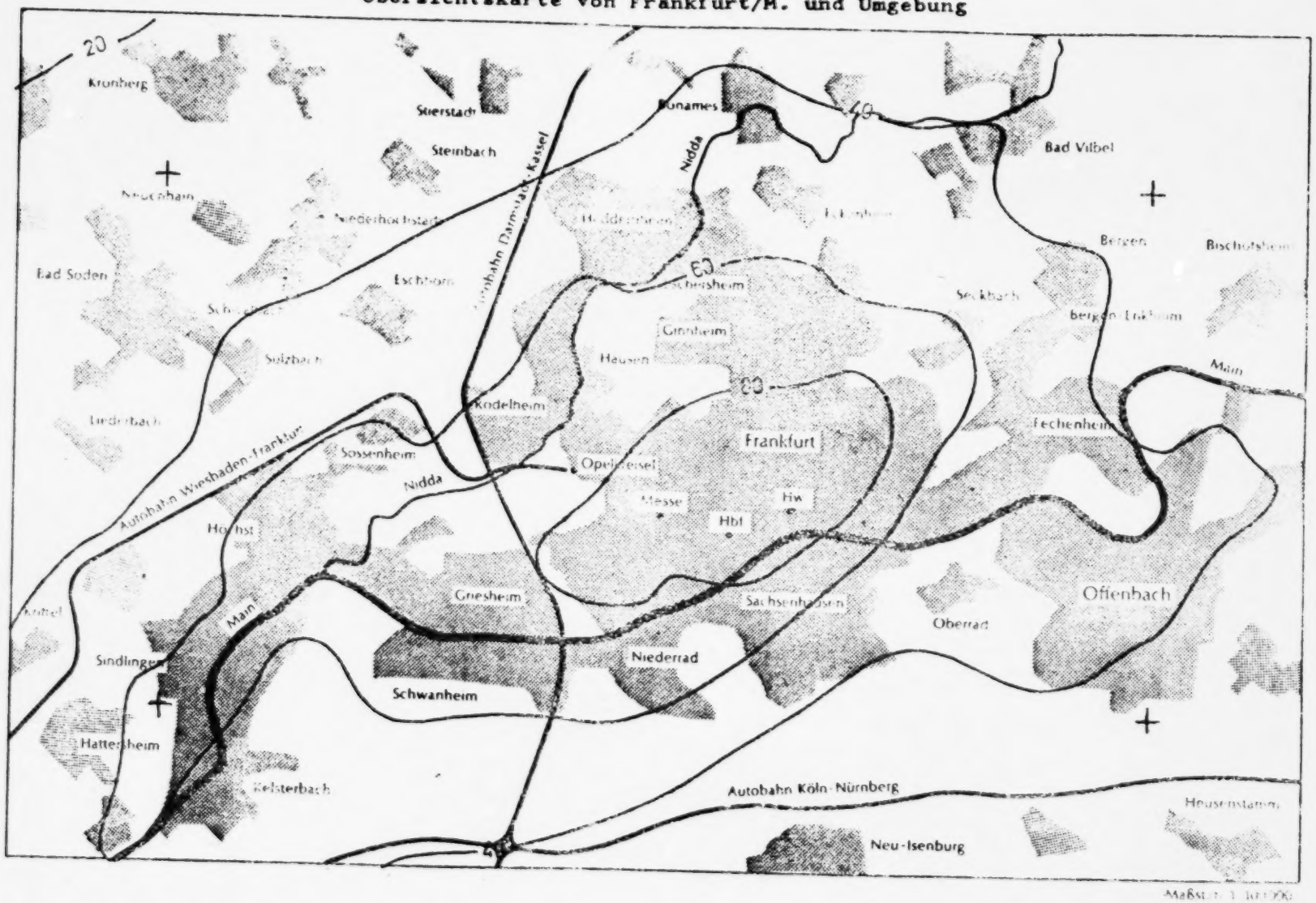

Figure 2 Model: KNMI

Calc. by: Nieuwstadt

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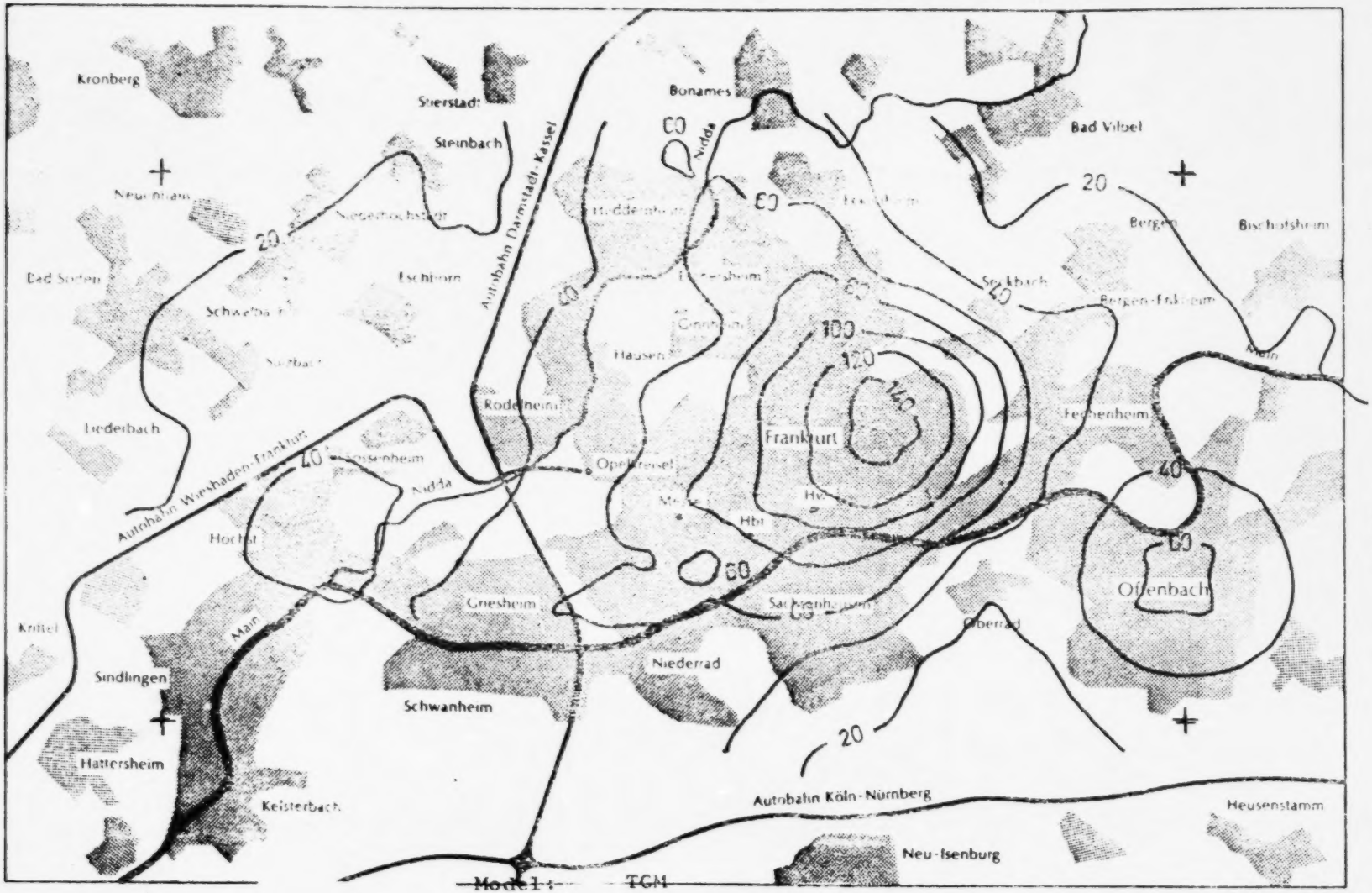

Figure 3 Calc. by: Christiansen, Porter

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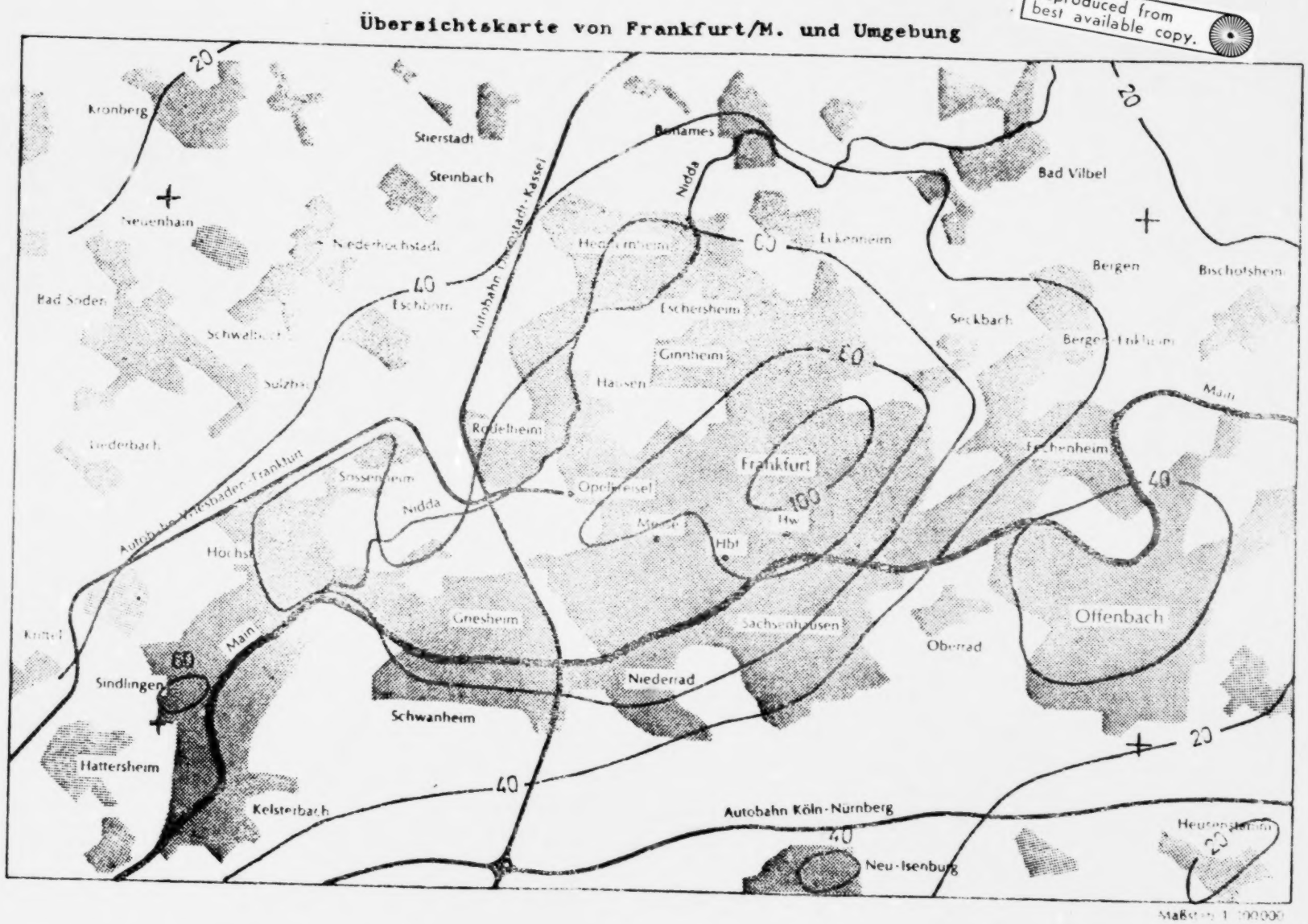

Figure 4 **Model:** TÜV-Rheinland

Calc. by: Kropp, Schneider (McElroy/Pooler a. Singer/Smith, Turner)

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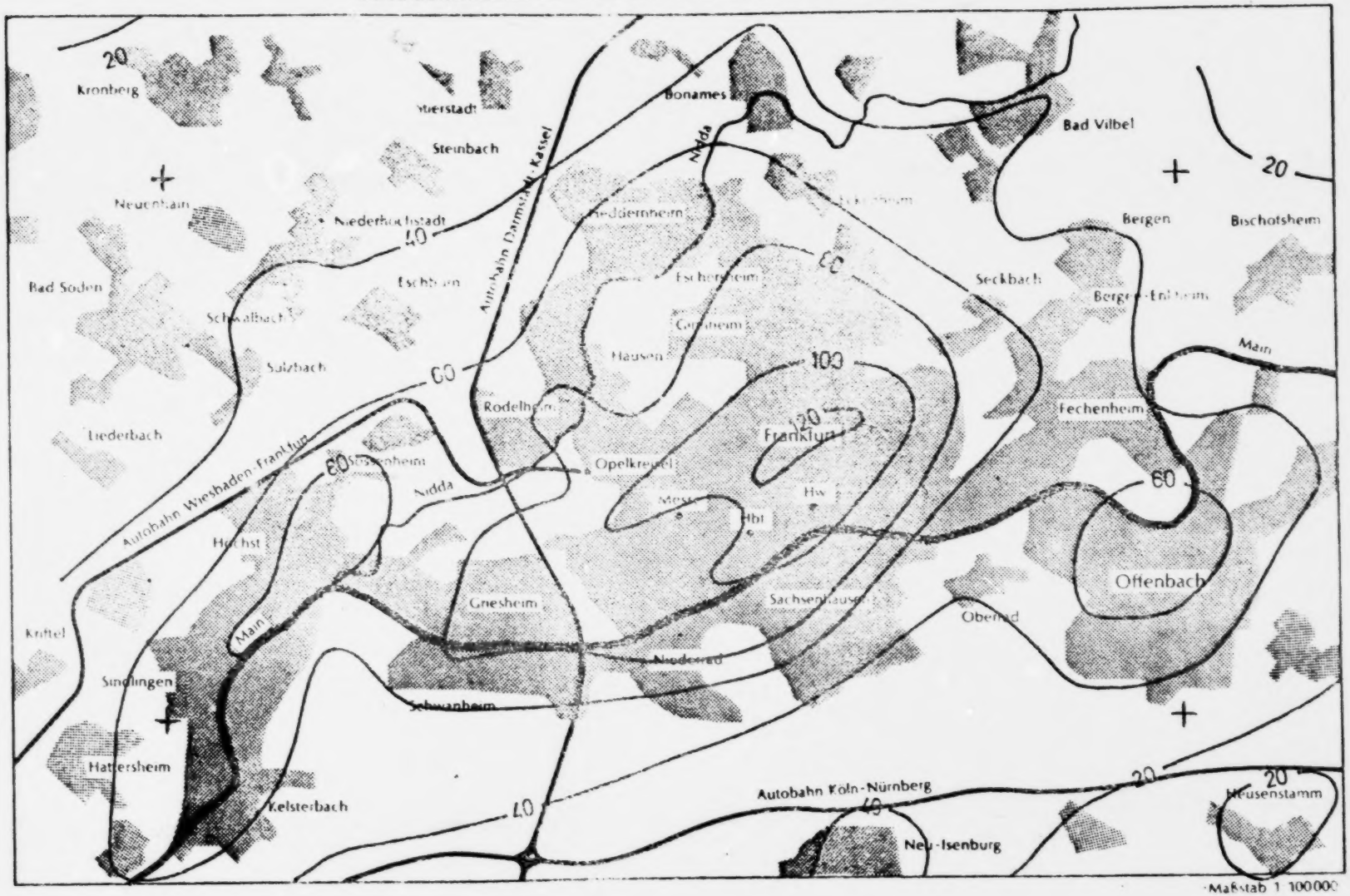

Figure 5 Model: TÜV-Rheinland

Calc. by: Kropp, Schneider (Polster/Vogt, Klug/Manier)

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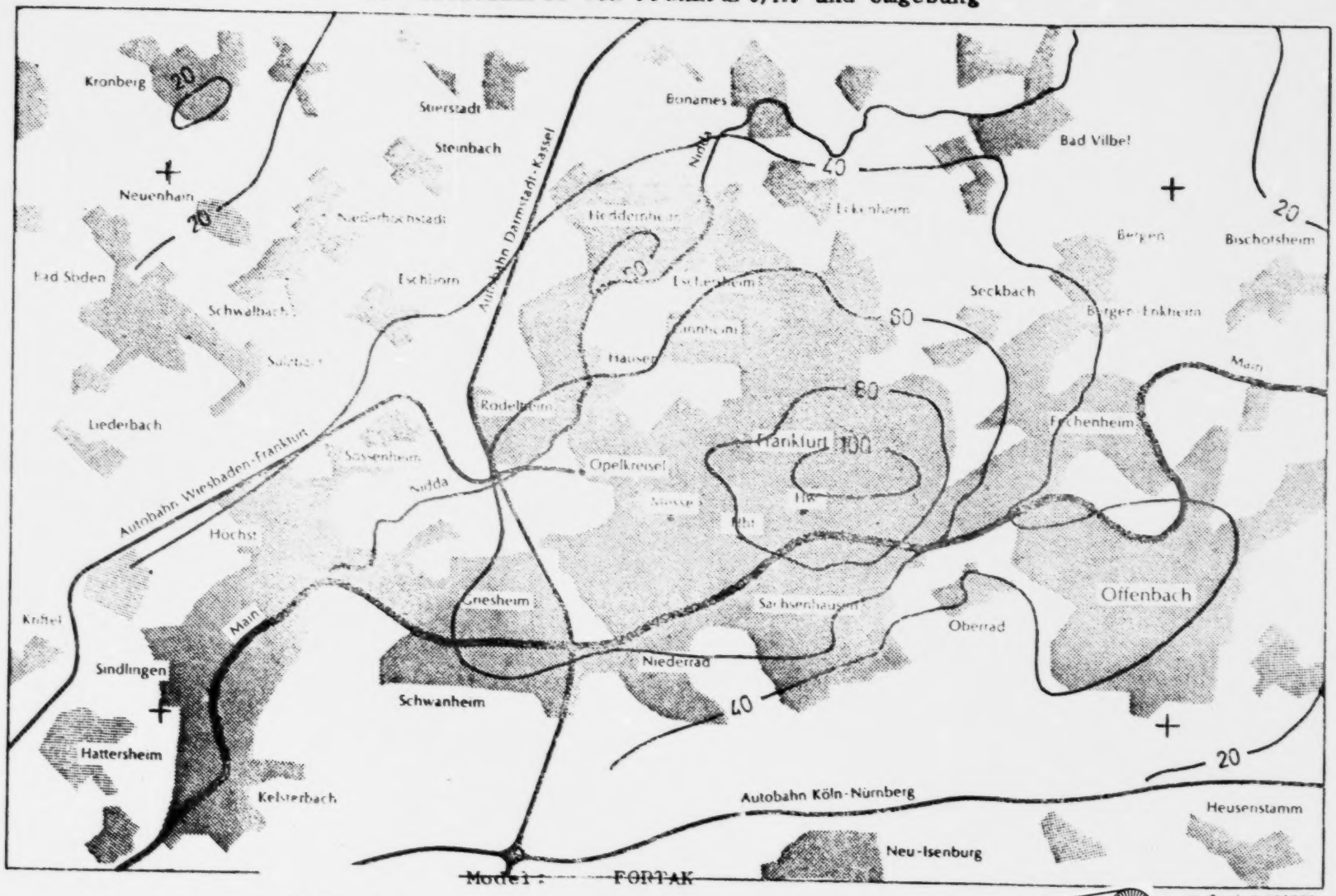

Model: ~~FORTAK~~

Figure 6 Calc. by: Stern, Gutsche, Timm

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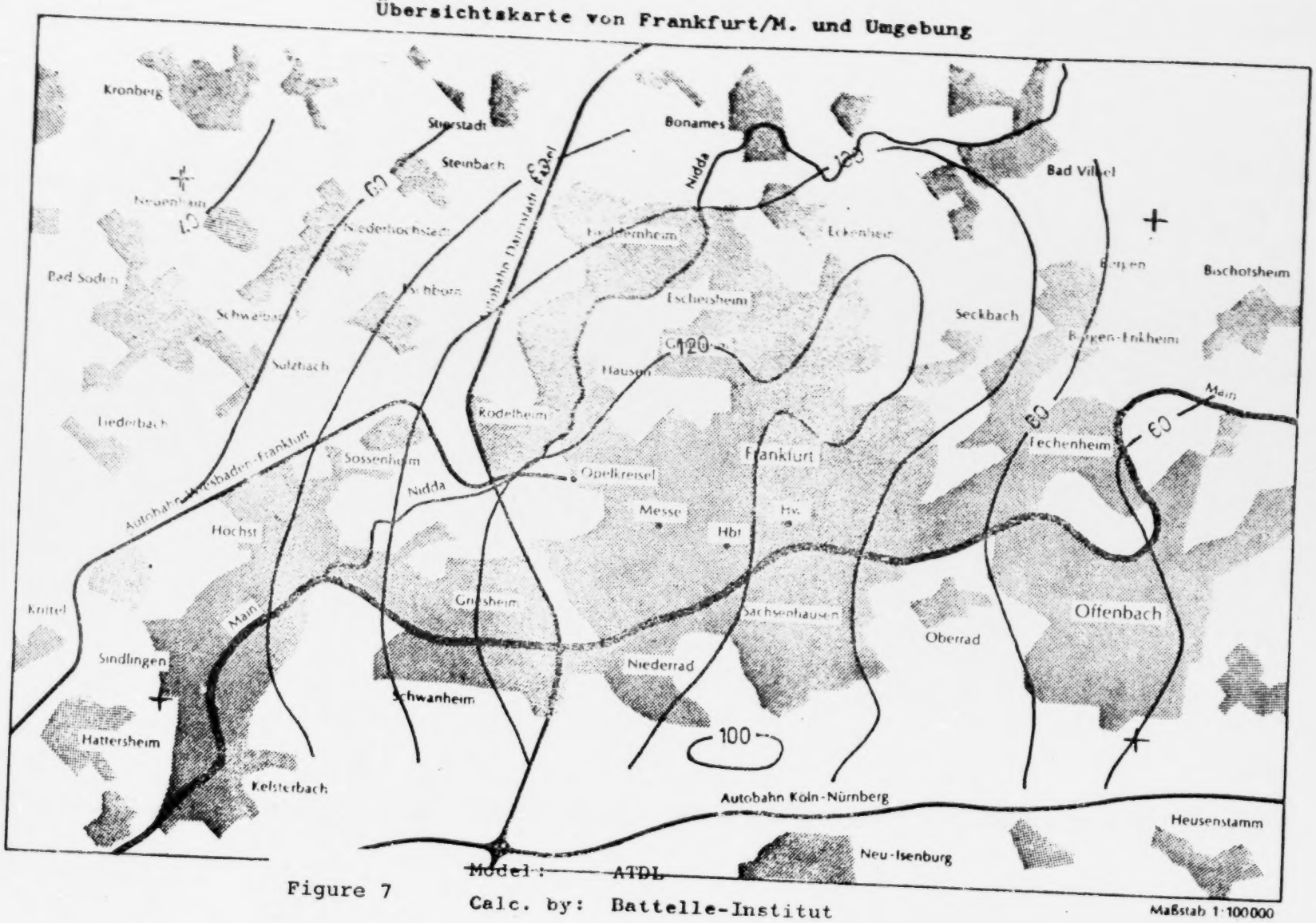

Figure 7

Model: ~~ATDL~~

Calc. by: Battelle-Institut

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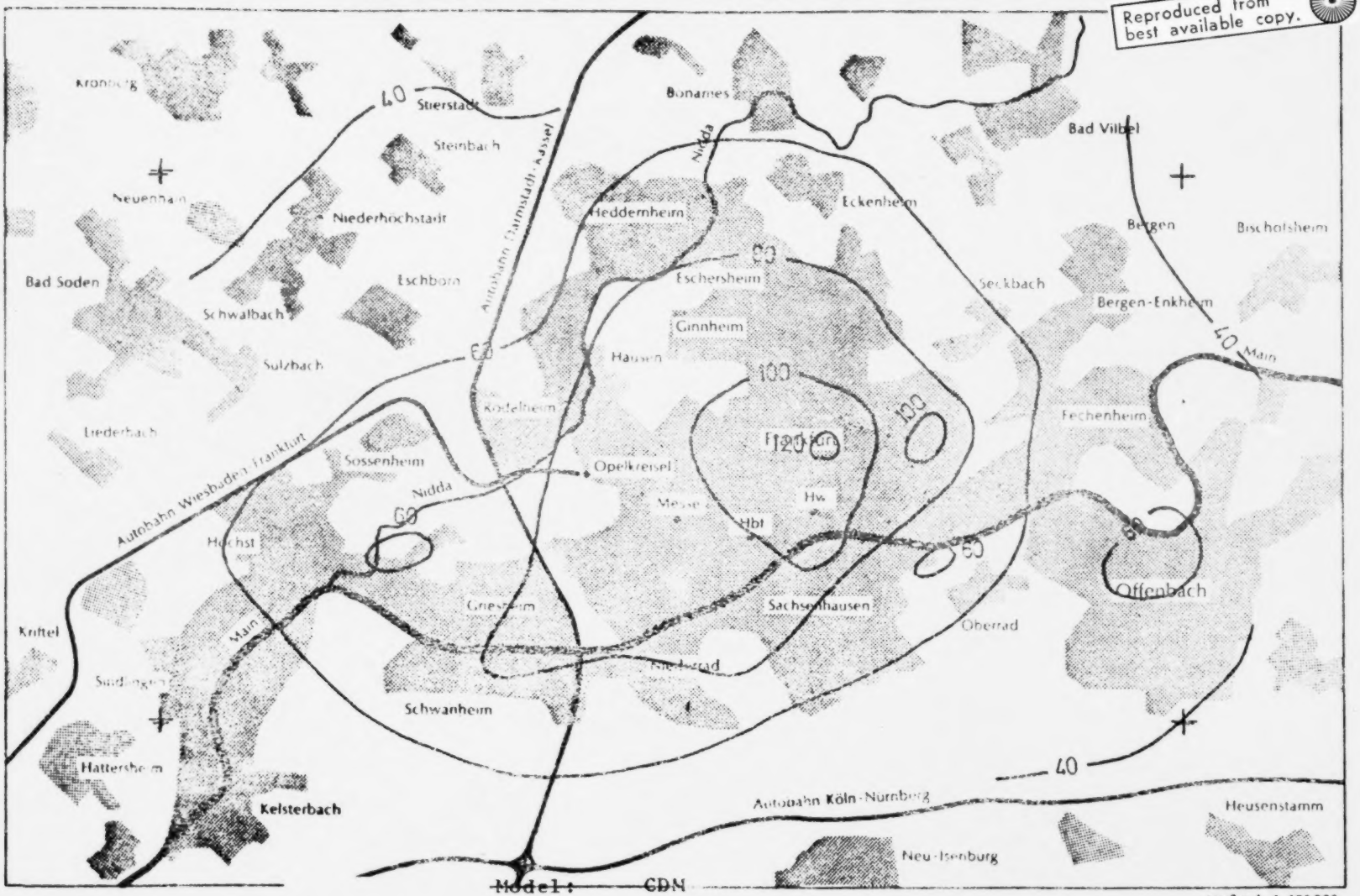

~~Model:~~ ~~CDN~~

Figure 8 Calc. by: Battelle-Institut

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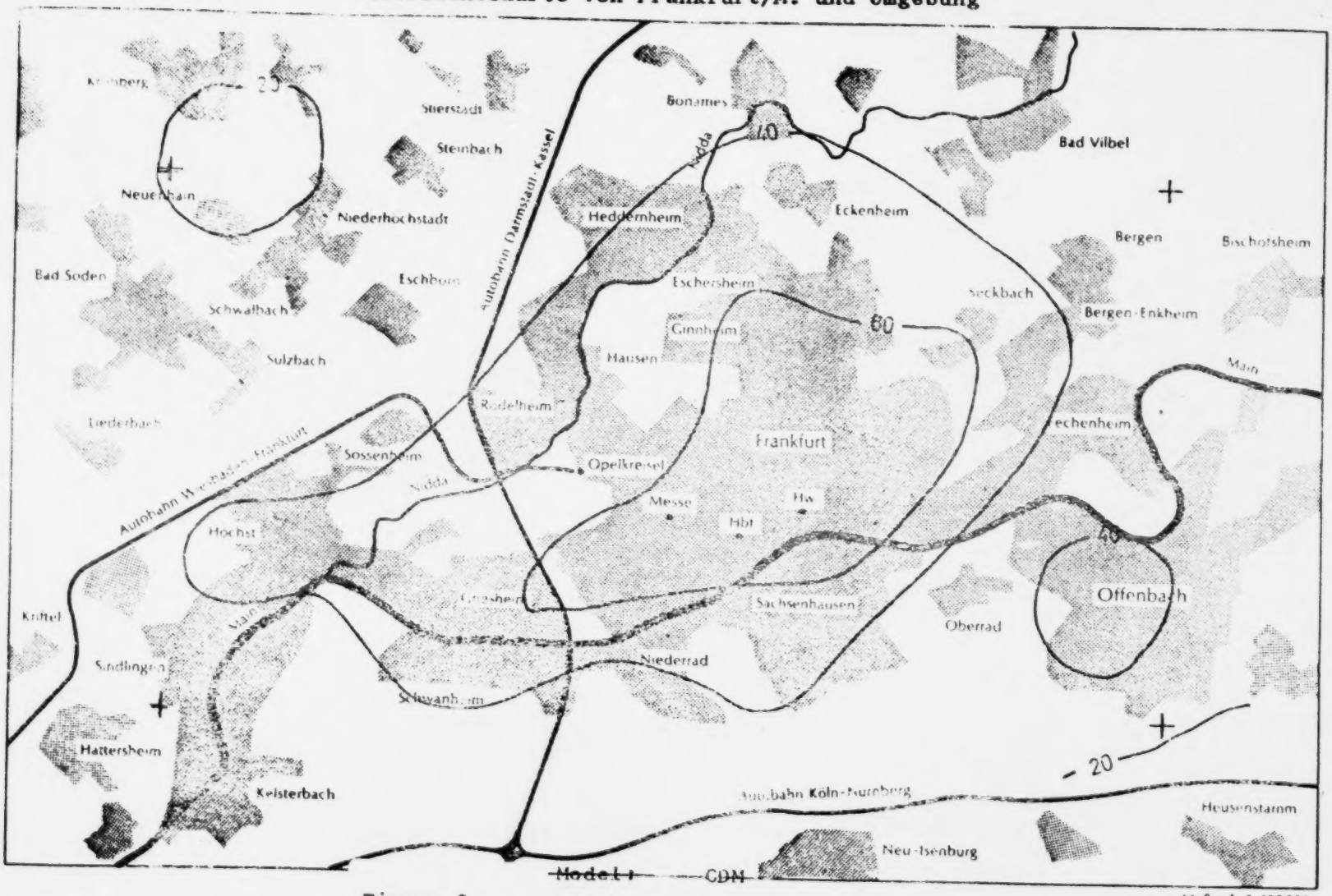

Figure 9 Calc. by: Turner

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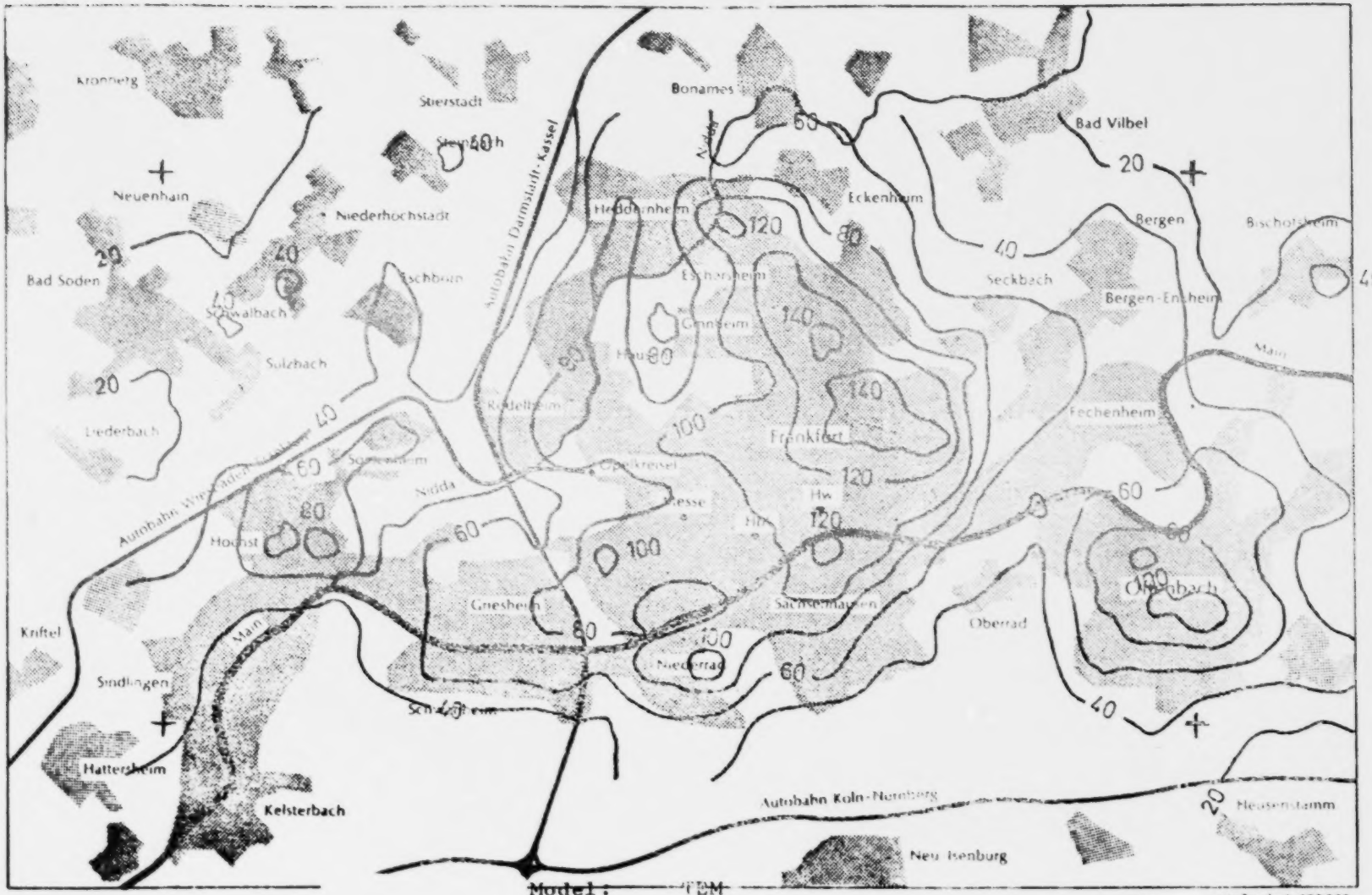

Figure 10

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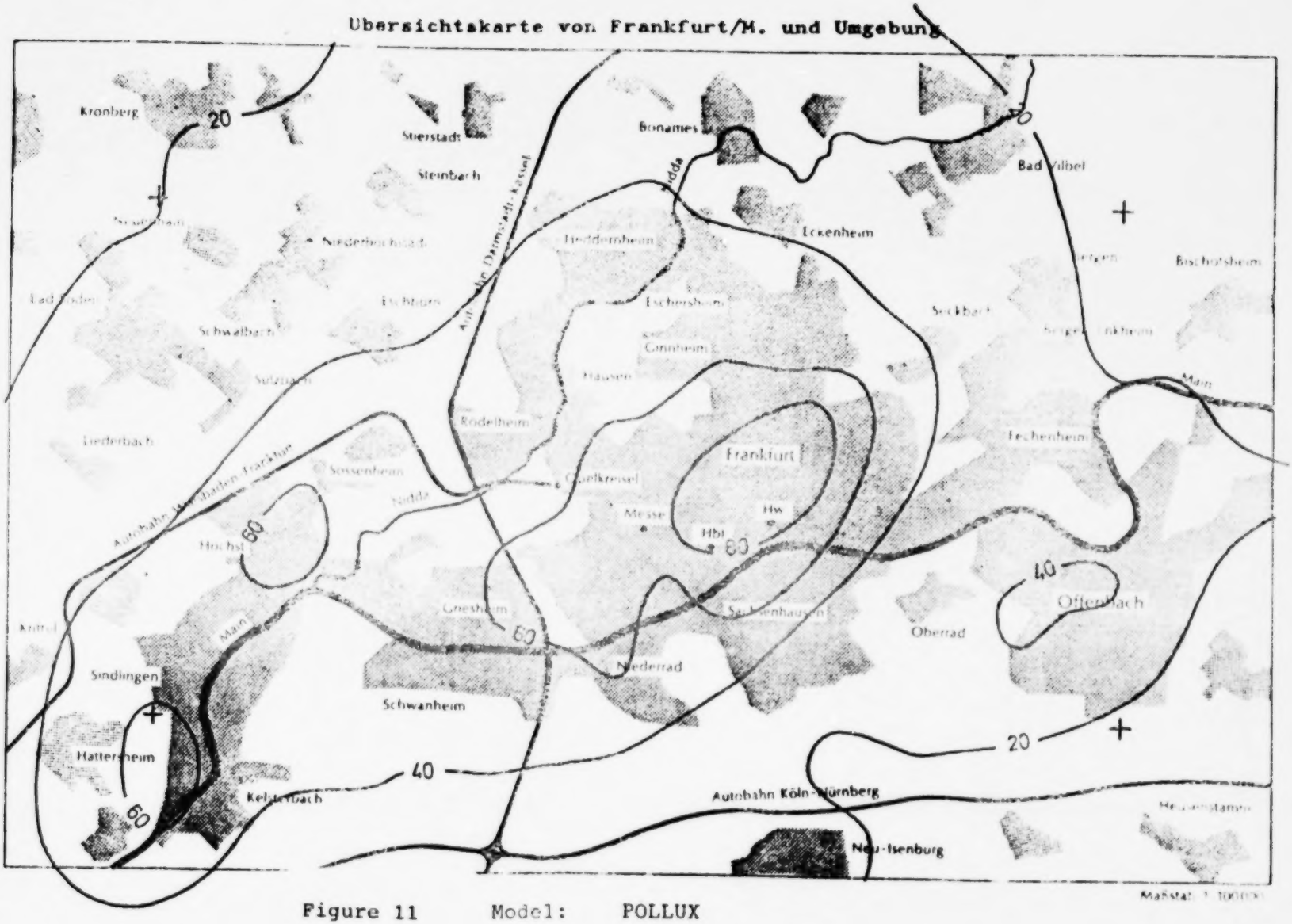

Figure 11 Model: POLLUX

Calc. by: Junod, Liechti

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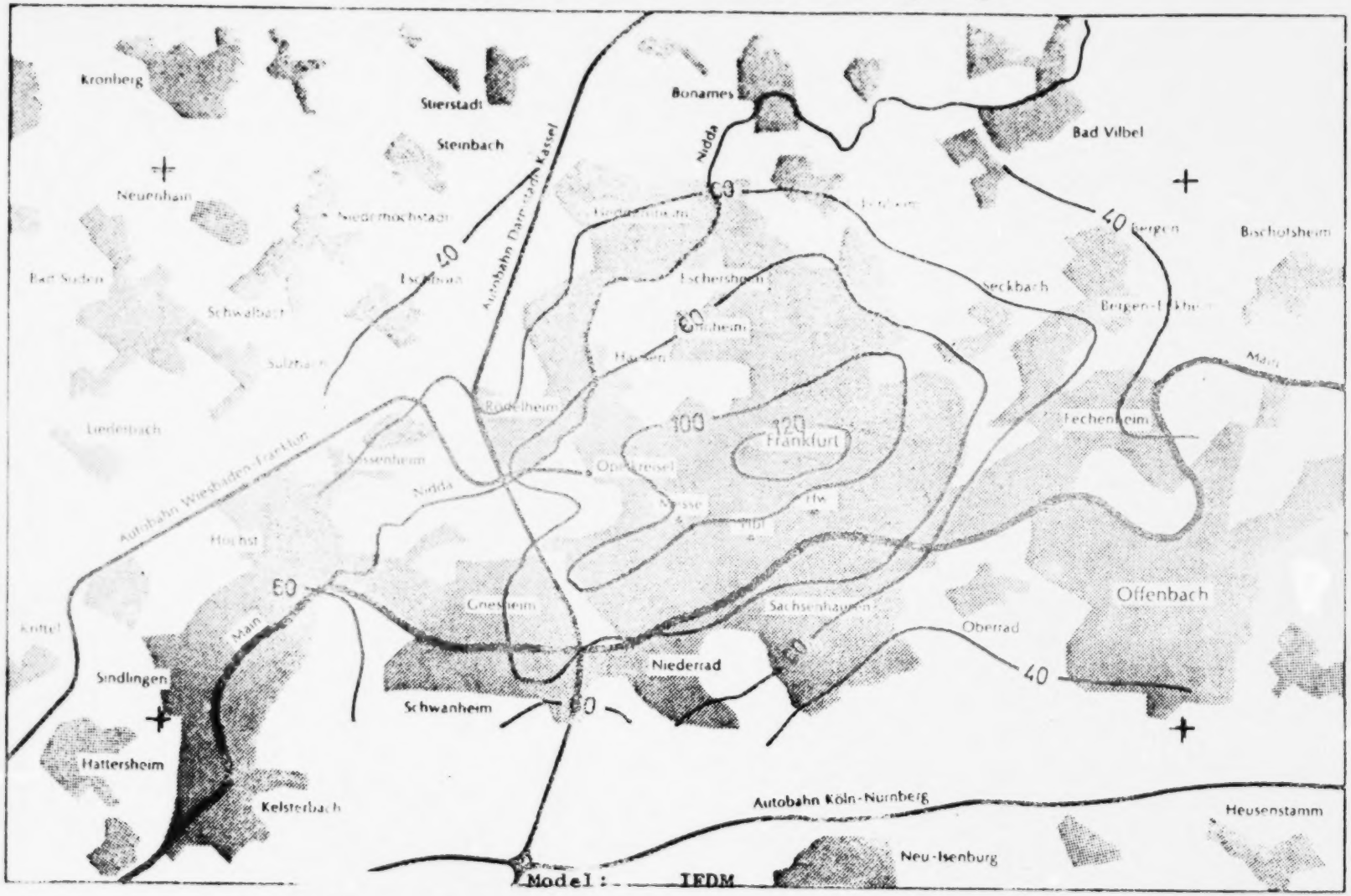

Figure 12 Calc. by: Kretzschmar

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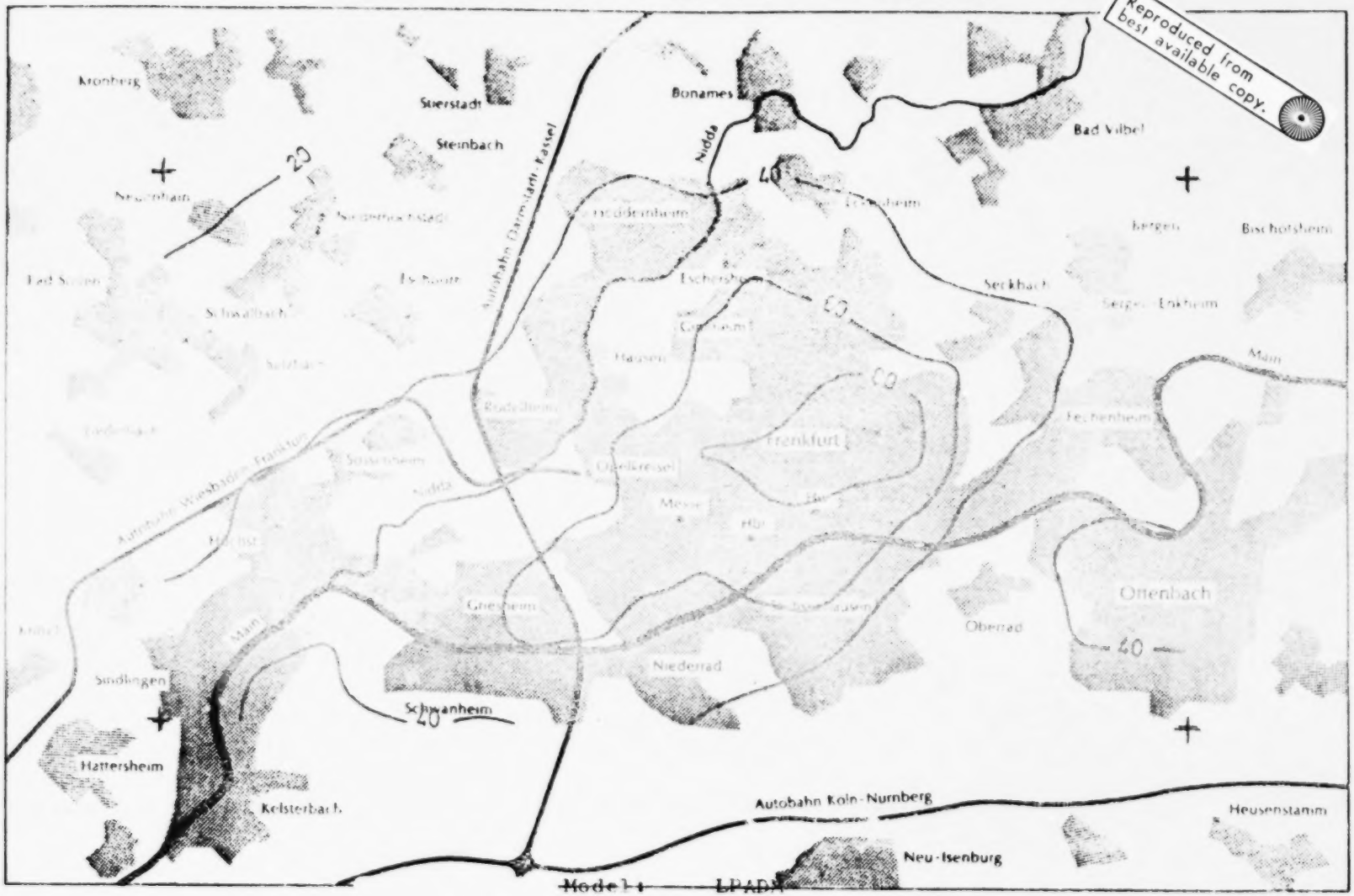
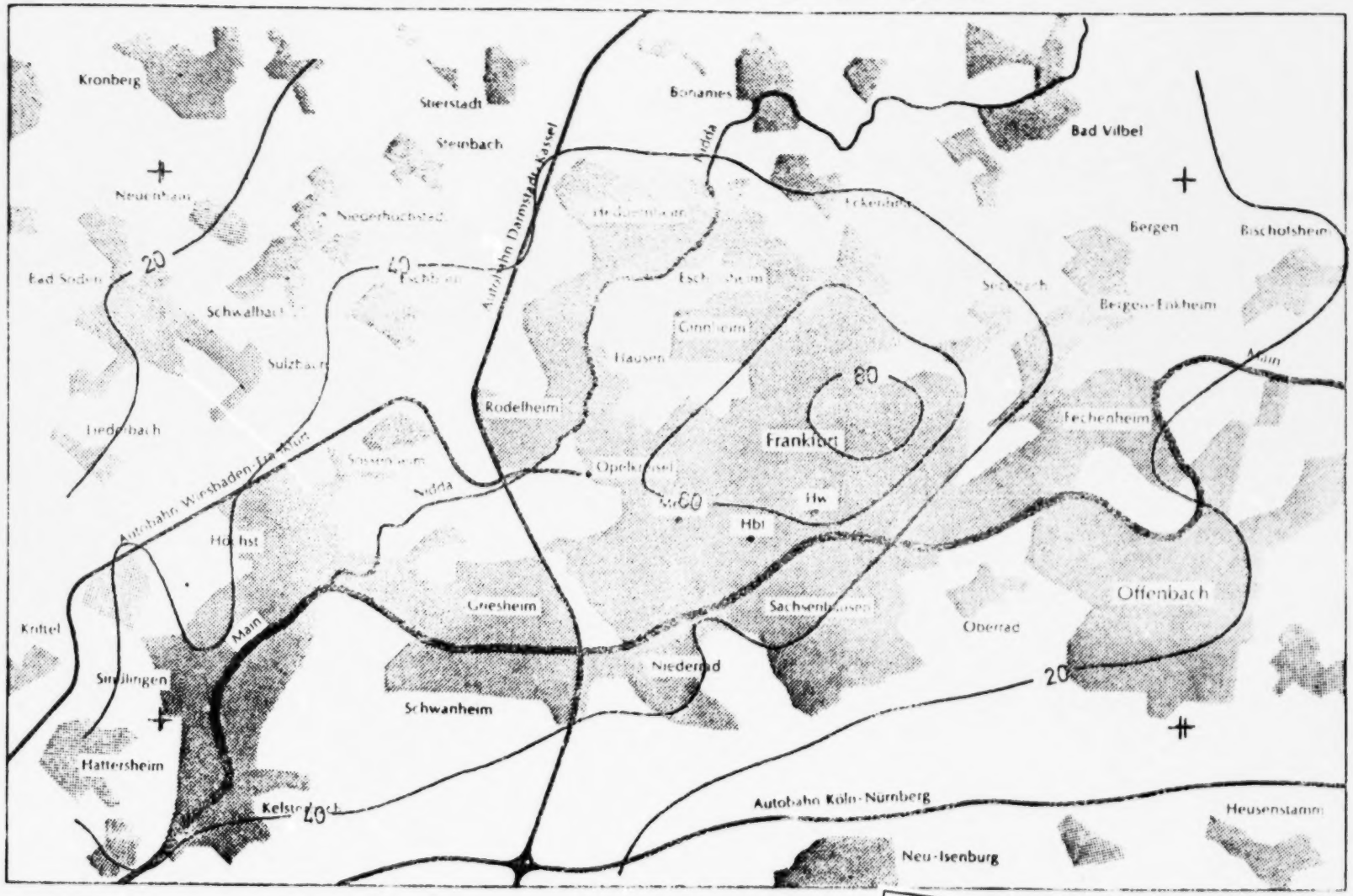


Figure 13 Calc. by: Berger

Model: LPADM

Maßstab 1:100000

Übersichtskarte von Frankfurt/M. und Umgebung



Maßstab 1:100 000

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Figure 14 **Model: KILDER**

Calc. by: Sivertsen

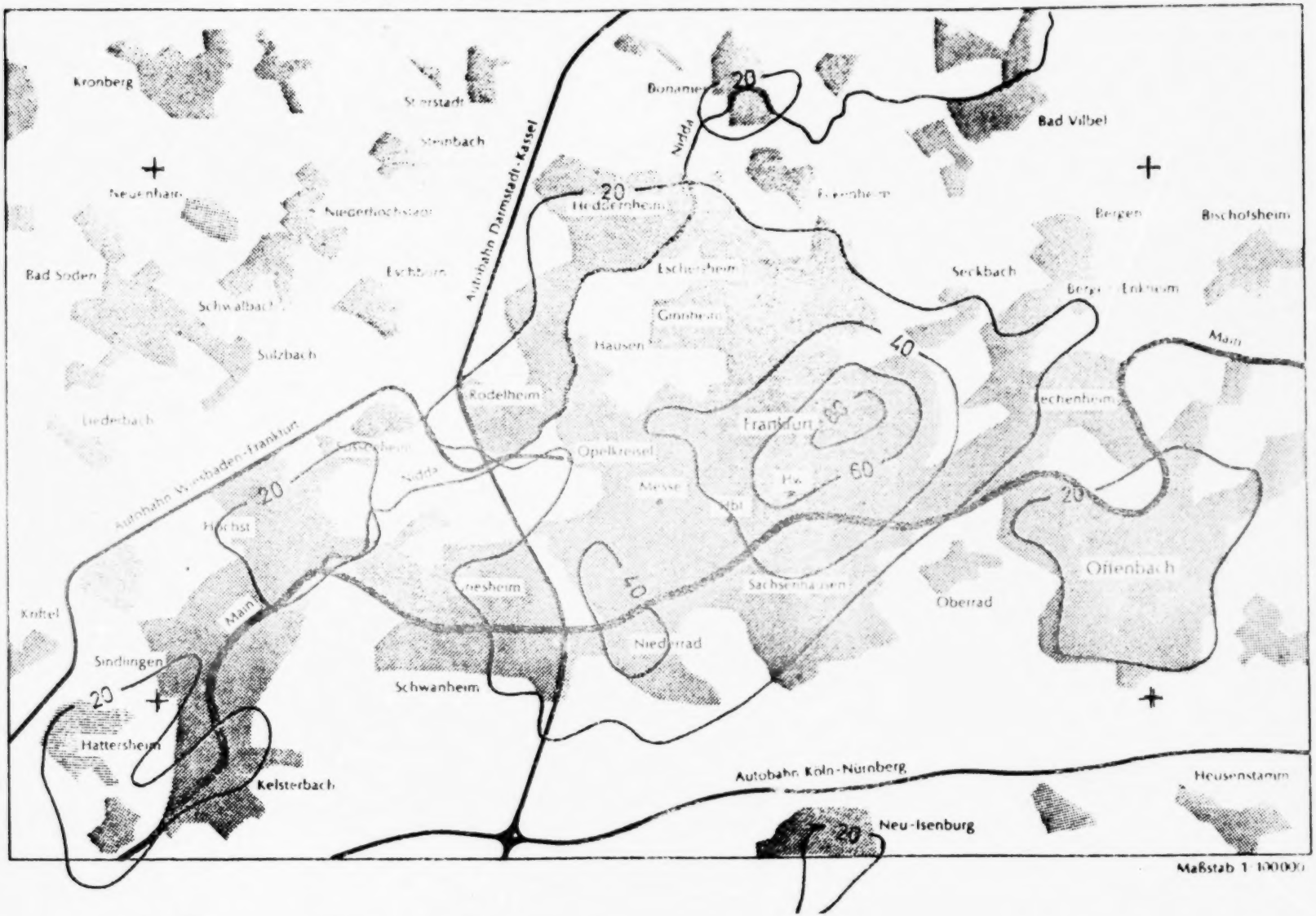

Figure 15 Model: ATDL/Milano

Calc. by: Santomauro, Tebaldi, Bellotti, Gualdi

Table 3: Calculated Annual Mean SO_2-Ground-Level-Concentration

Model	Calculation performed by	Receptor No. 1	2	3	4	5	6
Kilder	Schjoldager/Sivertsen	125,8	103,3	127,2	77,7	53,4	48,2
Fortak	Stern, Gutsche, Timm	66,8	99,0	81,0	52,4	38,0	42,1
KNMI	Nieuwstadt	78,5	65,1	88,3	70,1	44,8	41,4
SCAM	Irwin	71,72	56,6	75,2	47,32	21,29	37,85
CDM	Turner	68	59	71	50	29	35
CDM 36	Turner	71	60	76	53	30	37
CDM	Battelle	100,7	87,3	112,4	76,6	48,2	53,3
ATDL	Battelle	130,9	94,9	121,1	78,9	89,8	52,8
Kropp I	TÜV Rheinland	80	67	92	71	40	47
Kropp II	TÜV Rheinland	98	74	108	96	45	56
TCM	Texas Air Control Board	122,82	96,69	111,00	85,13	23,22	50,69
LPADM	Berger, Demuth Jacquart, Schayes	74	60	77	55	30	34
IFDM	Kretzschmar, De Baere Vandervee, Mertens	97	78	122	70	40	52
ATDL	Gifford, Hanna	60	120	110	30	10	30
Pollux	Junod, Liechti	62	57	79	57	37	28
ATDL/Milano	Santomauro	39,6	50,1	45,2	23,1	6,8	20,0

6.2 Comparison of the Model Results

A first classification of the results obtained by all these models can be made using a statistical analysis based on average concentrations, standard diviations and correlation analysis computed

- either for selected individual grid points or
- averaged over an ensemble of 36 or more grid points.

Such analyses have been performed by HANNA, by NIEUWSTADT, by BERGER and DEMUTH, and by GUTSCHE.

The results of these analyses were always quite similar and differed only gradually, sometimes strongly depending on the number of model results being available at the respective time of evaluation.

GUTSCHE evaluated statistically the model results at the 6 selected receptor sites cited above with the result of

- models of similar structure and comfort yield comparable concentration fields and maxima differed in the order of 20 to 30 percent in the annual mean value
- models using sector averaging (e.g. narrow-plume-hypothesis) seem to unterestimate the effect of singular emittents
- the correlation between more complicated model types and ATDL-model types is lower than the correlation between the other models among each other.

The Battelle-version of the ATDL-model even does not show a significant direct (or meteorology modified) relation between emission and immission field structure of the annual mean ground-level concentrations.

Quantitatively the results of this statistical analysis are shown in table 4. These results can be interpreted as follows:

- the calculated standard deviations are in the order of less than 30 % with respect to the annual mean value $\bar{x}_m$ (which means the arithmetical mean value of $\bar{x}_j$ for all models and for only one receptor point); the only exception is receptor point 5 with the lowest annual mean concentration values having a standard deviation of about 50 % with respect to $\bar{x}_m$.

  Absolutely the standard deviation is 20 to 25 µg/m³; only receptor point 6 has a lower standard deviation of about 10 µg/m³

- deviations greater/less than 2s or s, respectively are shown in the following tabulation:

Model	Number of Deviations within x and			
	x + s	x - s	x + 2s	x - 2s
Sivertsen	3	-	-	-
Stern/Gutsche/Timm	1	-	-	-
Nieuwstadt	-	-	-	-
Irwin	-	-	-	-
Turner/CDM	-	-	-	-
Turner/CDM 36	-	-	-	-
Battelle/CDM	1	-	-	-
Battelle/ATDL	3	-	1	-
Kropp I	-	-	-	-
Kropp II	2	-	-	-
Texas/TCM	2	-	-	-
Berger/LPADM	-	-	-	-
Kretzschmar/IFOM	1	-	-	-
Gifford/ATDL	1	-	-	3
Junod/Liechti	-	1	-	-
Santomauro/ATDL	-	4	-	2

Table 4: Statistical Analysis of Model Results

Model	No. of Receptor Sites 1	2	3	4	5	6	$\bar{x}_1$	s
Sivertsen	126*	103*	127*	78	53	48	89,2	34,9
Stern, Gutsche	67	99*	81	52	38	42	63,2	23,8
Nieuwstadt	79	65	88	70	45	41	64,7	18,6
Irwin	72	57	75	47	21	38	51,7	20,7
Turner/CDM	68	54	71	50	29	35	52,0	17,3
Turner/CDM 36	71	60	76	53	30	37	54,5	18,3
Battelle/CDM	101	87	112	77	48	53	79,7	25,6
Battelle/ATDL	131*	95	121*	79	90+	53*	94,8	28,3
Kropp I	80	67	92	71	40	47	66,2	19,7
Kropp II	98	74	108	96*	45	56*	79,5	25,3
Texas/TCM	123*	97	111	85*	23	51	81,7	37,9
Berger/LPADM	74	60	77	55	30	34	55,0	19,7
Kretzschmar/IFDM	97	78	122*	70	40	52	76,5	29,9
Gifford/ATDL	60	120*	110	30*	10*	30*	60,0	45,6
Junod	62*	57*	79*	57	37	28*	53,3	18,3
Santomauro/ATDL	40*	50*	45*	23+	7*	20+	30,8	16,7
$\bar{x}_m$	84,3	76,4	93,4	62,1	36,6	41,6		
s	26,0	21,2	23,2	19,7	19,3	10,5		
$\bar{x} - 2s$	31,4	30,2	44,0	23,2	-2,0	20,5		

$\bar{x}$ calculated annual mean ground level concentrations ($\mu g/m^3$)

s standard deviation ($\mu g/m^3$)

$\bar{x}_1$ arithmetical mean of $\bar{x}_i$ over all receptor points for one model

$\bar{x}_m$ arithmetical mean of $\bar{x}_j$ over all models for one receptor point

* deviations greater than $\bar{x}_m \pm s$

\+ deviations greater than $\bar{x}_m \pm 2s$

This statistical analysis was the basis for the statements given above. It has to be mentioned once more that this does not represent a model validation, but only a comparison between different model results. A similar analysis has been performed by BERGER and DEMUTH.

The first impression, which will be emphasized later by the comparison with measurements, is that a grouping into two classes of model types can be made:

- complicated and relatively "expensive" models (with respect to required core and computing time), showing all nearly the same quality of model results
- simple models, which can easily be handled on a desk computer, giving a quick overview over the general air pollution situation, making allowance for larger deviations in special locations.

There are at least three objections which could be made against this interpretation

- the receptor points chosen for model comparison are not representative for the whole "Test-City", an aspect, which will be investigated in the following statistical analysis by NIEUWSTADT
- the number of more complicated models is clearly dominating the number of the second group of more simple models in such a way that both groups are not treated in a statistically unique manner.
- it is not at all true that the overall average of a number of individual (not validated) model calculations is closer to reality than whatever individual result. Therefore, this is not an evaluation of the model results but a discussion of the range of results.

Only a direct comparison with a comparable set of measured data will yield a reasonable interpretation of model results and a model validation as a mathematical-meteorological basis for air quality management and regional planning activities as well e.g. for licensing procedures.

NIEUWSTADT constructed a grid of 36 points in the area of Frankfurt, chosen in such a way, that mainly the region of highest occuring concentrations were considered. Since values of the annual mean ground-level concentration were not available at these gridpoints for all these models, they were derived from an interpolation by eye of the concentration patterns.

The average m and the standard deviation s over the 36 selected gridpoints in the city-center for each model is given in table 5. The average m indicates the average concentration level in the area. For most of the models, except two ATDL-type models, this average is about (60 $\pm$ 15 $\mu g/m^3$).

Table 5: Statistical Analysis of Nieuwstadt

Model	m ($\mu g/m^3$)	s ($\mu g/m^3$)
1. Kretzschmar/IFDM	65	21
2. Stern, Gutsche, Timm, Fortak	57	18
3. Christiansen, Porter/TCM	54	28
4. Christiansen/TEM	68	28
5. Battelle-Institut/ATDL	108	14
6. Battelle-Institut/CDM	72	16
7. Turner/CDM	47	12
8. Berger/LPADH	48	15
9. Kropp, TÜV Rheinland	58	18
10. Nieuwstadt/KNMI	60	16
11. Sivertsen, Kilder	45	15
12. Santomauro/ATDL	27	14

The standard deviation indicates the amount of variance in the concentration patterns. For most of the models the standard deviation calculated for the selected 36 grid points is about 17 $\mu g/m^3$.

In the following table the correlation matrix of the values at the gridpoints of all the models is given (after NIEUWSTADT):

models	1	2	3	4	5	6	7	8	9	10	11
1											
2	.88										
3	.86	.88									
4	.86	.84	.91								
5	.67	.48	.44	.45							
6	.94	.86	.84	.84	.67						
7	.93	.90	.87	.87	.61	.91					
8	.94	.89	.89	.90	.60	.94	.95				
9	.94	.86	.88	.89	.66	.92	.94	.96			
10	.95	.85	.77	.76	.71	.93	.90	.91	.91		
11	.88	.77	.82	.81	.59	.80	.84	.87	.92	.84	
12	.78	.83	.91	.84	.40	.81	.79	.87	.80	.73	.72

The correlation coefficient of the results of two models indicates how much the variations with concentration patterns ressemble each other. Especially, the ATDL-version by Battelle compares unfavourably with all other models. It is of interest that this statement also holds for the correlation between the Battelle ATDL-version and SANTOMAURO's ATDL-version, a result showing once more that already small individual changes of an available model code may lead to substantial effects in the model output. This is also true for all other model types,

as can be seen in the sensitivity analyses for dispersion parameters and plume rise formula in the next chapter. As a consequence, it has to be noted that only model changes on a physically and meteorologically sound basis can lead to improvements in model results.

Concerning the evaluation procedure mentioned above three remarks have to be made:

- due to the choice of plume rise formula and dispersion parameters, the smoothing effect in the concentration patterns differs from one model to the other; therefore, a statistical analysis in the sense cited above may only yield a first but very instructive approximation in model comparison
- due to the choice of only 36 grid points in the region of the highest concentration values, the city center-suburb concentration gradient (see GUTSCHE and LENSCHOW (1973)), being typically too large for most of the Gaussian plume models, cannot be taken into consideration
- because the form of the model output had not been prescribed in the "Practical Demonstration", the bandwidth of concentration pattern analysis (concentration isoplets) ranges from detailed hand analysis over numerical analysis up to zebra analysis, leading (taking into account numerical filter theory) to quite different smoothing effects.

Concerning the second point it has to be investigated how far the immission-climatological concept built up of 1/2 - or 1 - hourly meteorological situations being (in theory) totally separated from one another is suitable for des-

cribing such a large concentration field which is characterized by air pollution transport from surrounding places, by local circulation systems, by meso- and large-scale diffusion effects, by roughness changes and so on. The simplest method, which in the statistics of an annual mean concentration value seems to give reasonable results in the surrounding of a city-center, appears to be GIFFORD and HANNA's estimation of background concentrations (see part II of this document).

Considering the third point of the list above the conclusion has to be drawn that in a "Practical Demonstration of Urban Air Quality Simulation Models" kind and form of the model output has also to be described to make conformity and differences between model results more transparent and to enable a more objective evaluation and interpretation.

All these statistical comparisons have been performed for the annual mean ground-level concentration. The large differences with respect to the 95 percentile or with respect to the whole cumulative frequency distribution did not allow a reasonable analysis. To get an impression of the extremely broad spectrum for different models in higher percentiles refer to the detailed results published in Part II of this document.

6.3 Sensitivity Analysis

Based on the suggestions made on page 33 of this document, sensitivity analysis involves an investigation of the relationships between changes in selected independent quantities and the corresponding resulting changes in specific dependent model outputs.

The main types of performing a sensitivity analysis have also been presented in chapter 5 of this document. We may summarize the procedures as follows (after D. ROTE):

Given a quantity f, that is a function of several (here N) independent quantities, x_1, x_2, x_3, etc., the maximum expected percent error in f can be expressed approximately as

$$\Delta f \approx f \sum_{i=1}^{N} \frac{\ln f}{\partial x_i} \Delta x_i$$

where $\frac{\partial \ln f}{\partial x_i}$ represents the partial derivative of the natural logarithm of f with respect to x_i, and Δx_i is an estimate of the expected error in x_i. The partial derivatives are measures of the sensitivity of f to the corresponding independent variables x_i. This is, of course, only a first order estimate since the response of f to a change in x_i of order Δx_i may be nonlinear in Δx_i.

These partial derivatives reflect the main characteristics being inherent in the presuppositions for the ground-level concentration field being a bivariate GAUSSian distribution; on the other hand, it has to be stated, that many of these parameters are interrelated. Therefore, the differentials $d P_i / d P_j$ for each have to be developed (for further details see PORTER and WOLBACH (1975)).

As an illustrative example the expected error in concentration at a given site is calculated on this basis when there is an error dx in the downwind distance x from the source to the receptor, assuming power laws

$$\sigma_z = A\, x^B \qquad \sigma_y = C\, x^D$$

for the dispersion parameters.

The result, then, is:

$$\frac{ds}{dx} = s \left(\frac{D}{x} \left(\frac{y^2}{\sigma_y^2} - 1\right) + \frac{B}{x} \left(\frac{h^2}{\sigma_z^2} - 1\right)\right)$$

which is in quite good agreement with measurements and numerical calculations for single sources.

The interrelation between several kinds of parameters can be expressed by a short view upon the list of only some GAUSSian plume model (see Chapter 3), those, which have participated in the "Practical Demonstration of Urban Air Quality Simulation Models". In this way, the variety of e.g. different combinations between plume rise formulas, sets of dispersion parameters, and stability classification schemes can easily be demonstrated (see Chapter 3), illustrating the well-known negligence - due to reason of practicability - of the mutual dependency of such meteorological parameters.

In spite of the functional connection between dispersion parameters and stability classification scheme, which has been pointed out by NIEUWSTADT (1975), relatively arbitrary connections between these two factors have been used in most of these models. The bandwidth, which can be caused by such a procedure, is demonstrated in the figures 17 and 18. These figures show the calculated annual mean SO_2-ground-level concentration for a power station with a physical stack height of 110 m. The meteorological data of Frankfurt have been used, which are characterized by a pronounced North-East- and South-West - orientation and a high frequency of stable situations. Figure 17 shows the concentration field calculated with the dispersion parameters by Singer and Smith and the plume rise formula by Moses and Carson. Figure 18 shows the correspond-

ing concentration field using the dispersion parameters from the Jülich experiments and the plume rise equation by Briggs. Differences of the order 2 to 3 even in the annual mean value are present (for these calculations FORTAK's model has been used).

Due to the multiple-source character of urban dispersion models the presence of a large variety of different emittents causes some statistical smeering-out, and the differences are no longer as high. This can be seen from figure 19. In the vicinity of an industrial area (south-west region of the city) the annual mean SO_2-ground-level concentrations due to all singular emittents with source strengths of more than 1 kg SO_2/h are about 50 % higher when being calculated with the Jülich dispersion parameters than those when making use of Singer and Smith's data. If additionally space heating, which represents 60 to 70 % of all SO_2-sources in the Frankfurt-area are taken into consideration, the differences reduce to 10 to 20 % in the total annual mean concentration field.

The differences, however, are again much more pronounced in the resulting cumulative frequency distributions for defined receptor sites.

Summarizing the results of this sensitivity analyses it can be stated, that due to the mutual dependency of data and parameters influencing the transmission process uncertainties in the calculated annual mean SO_2-ground-level-concentration values are in each case of order of about 20 or 30 % in multiple-source urban diffusion models and can increase to 2 or 3 orders in magnitude for single sourcres. Corresponding results were give by KRETZSCHMAR ET AL.

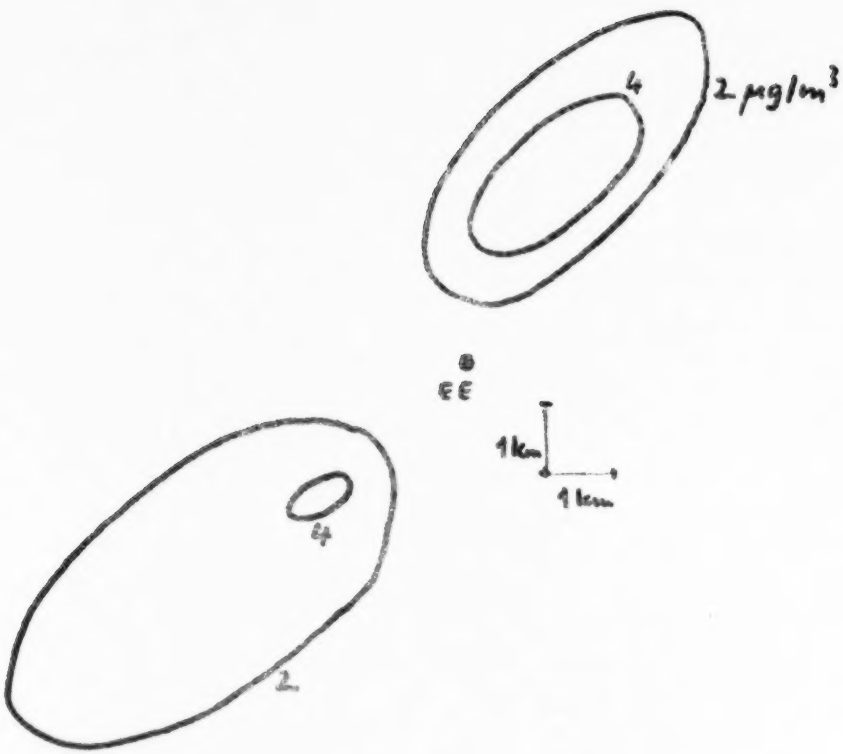

Figure 17: Calculated annual mean SO_2-ground-level concentrations due to a power station (physical stack height 110 m) using dispersion parameters by Singer and Smith and the plume rise formula by Moses and Carson

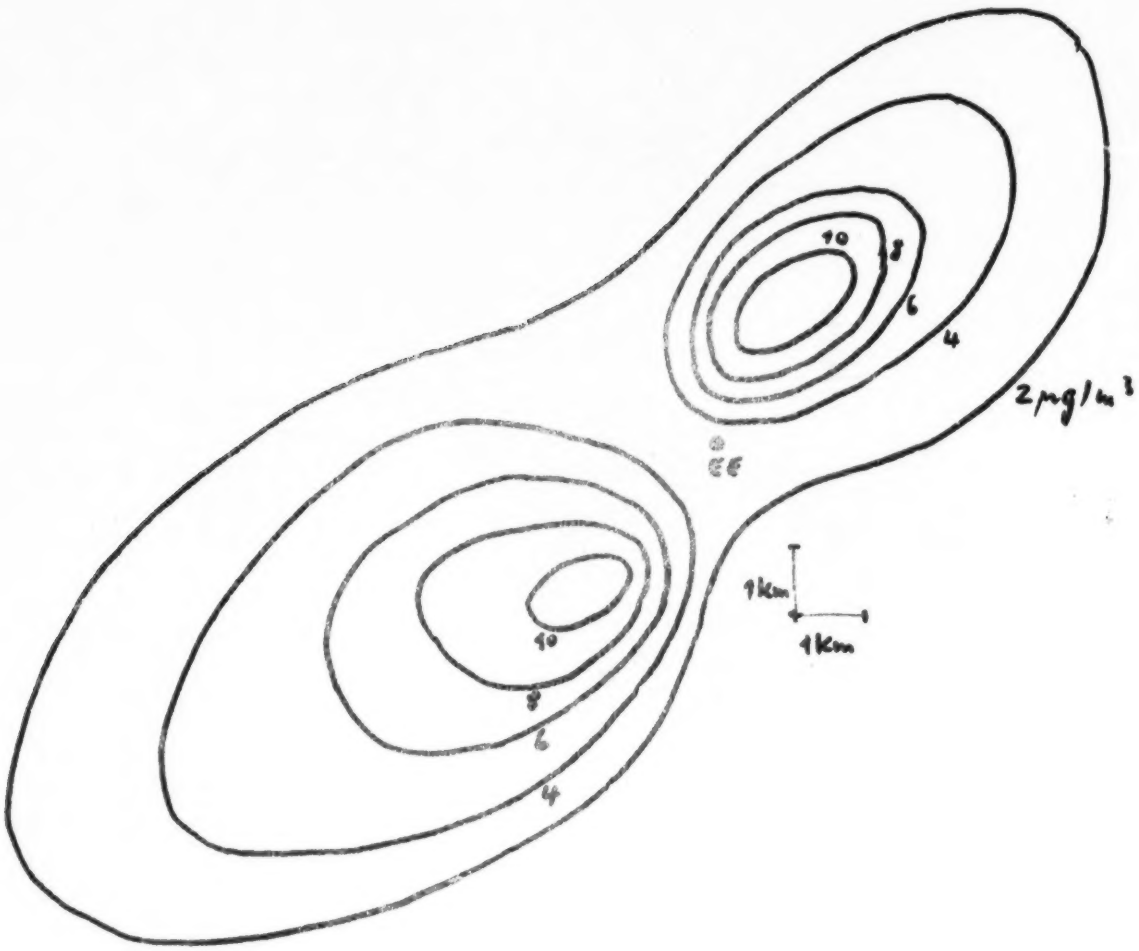

Figure 18: Calculated annual mean SO_2-ground-level concentrations due to a power station (physical stack height 110 m) using dispersion parameters from the Jülich experiments and the plume rise formula by Briggs

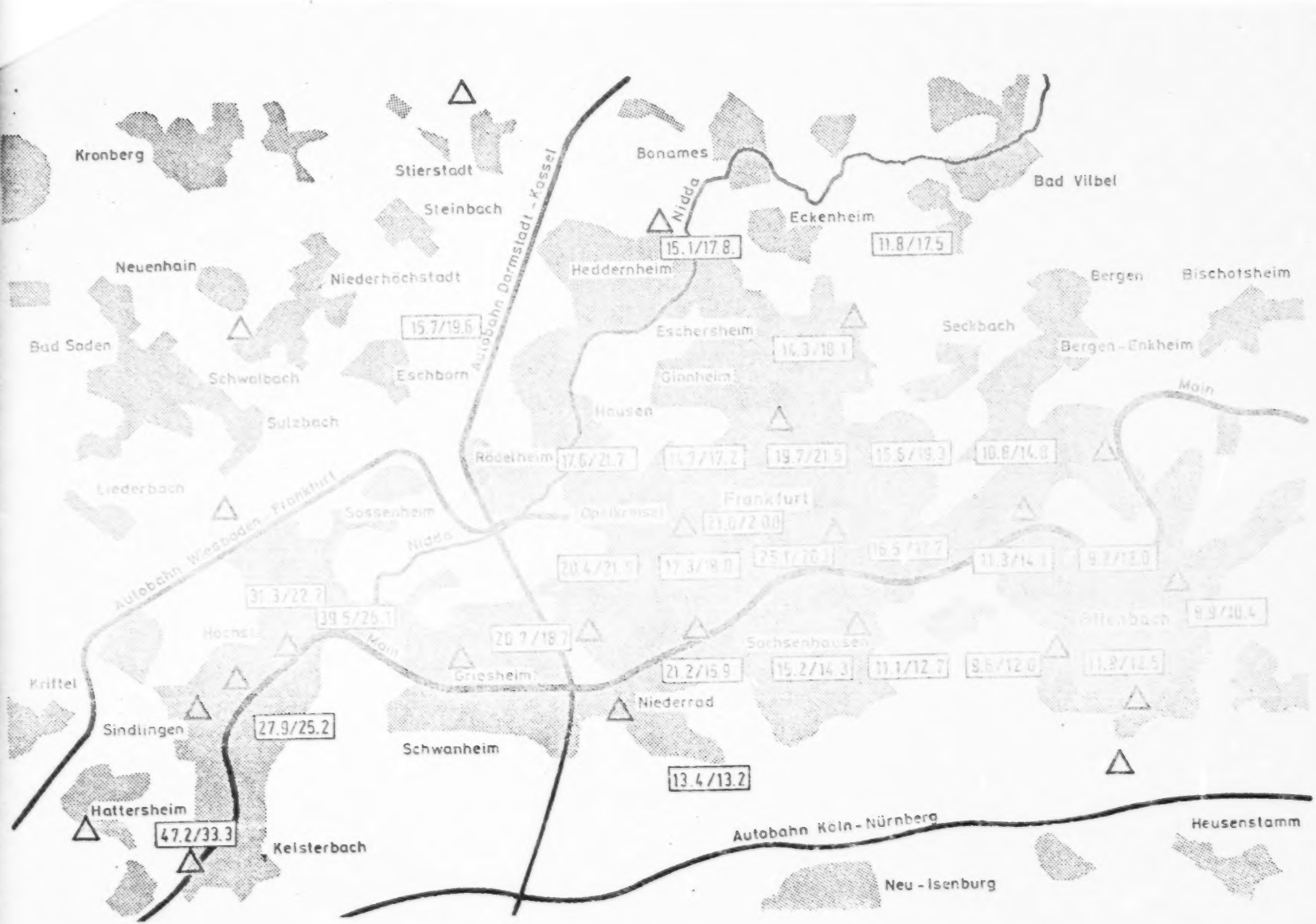

Figure 19: Calculated annual mean SO_2-ground-level concentrations (µg/m³) due to big singular emittents;
left number: using dispersion parameters from the Jülich experiments
right number: using SINGER and SMITH's dispersion parameters
triangles: position of some of the biggest singular emittents

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Mutual interdependencies of several different, non-linearly correlating parameters have not yet been investigated in a sufficient manner.

But in the sense of chapter 1 of this document such sensitivity analyses seem to be a necessary and suitable basis for model standardization.

7. Comparison of Calculated Model Results with available Measured Immission Concentration Data

In the Frankfurt area two kinds of SO_2-data are available

- from continuous, automatic measurements
- from random samples.

Continuous, automatic measurements are available for the following seven receptor sites:

Receptor-Site	GAUSS-KRÜGER Coord.	"Test-City"-Coord.
Zentralstation	347570; 555410	2470; 2910
Niedererlenbach	347890; 556220	2790; 3720
Nied	347010; 555250	1910, 2750
Offenbach	348100; 555260	3000; 2760
Hattersheim	346220; 554710	1120; 2210
Neu-Isenburg	347920; 554750	2820; 2250
Großkrotzenburg	349670; 555040	4570; 2540

where only the "Zentralstation" seems to have worked continuously for nearly the whole year, while the other stations only worked sporadicly. Furthermore, only the Zentralstation corresponds approximately with a receptor point in the regular grid used for the calculations. Therefore, this receptor-site seems to be the only continuously working measuring station where calculated and measured values can be compared in "stricto sense".

The measured annual mean SO_2 ground-level concentrations for the period from Aug. 1971 to July 1972 can be taken from the following table:

Receptor Site	Arithmetical mean	
	ppb	µg/m³
Zentralstation	46	132
Niedererlenbach	18	51
Nied	37	106
Offenbach	30	86
Hattersheim	13	37
Neu-Isenburg	16	46
Großkrotzenburg	21	60

Further details, especially

- the structure of the cumulative frequency distribution
- and the temporal (here monthly) course of immission concentrations

can be taken from Appendix II of this document.

The second kind of available SO_2-data, random measurements (as LAHMANN points out in NATO/CCMS Air Pollution No. 6 (Revised), 1977), were carried out manually having the advantages

- that specimen can be collected at practically any location
- that they are a favourable method for determining spatial immission distributions, at least of the annual mean value.

The main disadvantage is, however:

- the limited information on the temporal course of immission and on meteorological influences.

Another disadvantage is the limited information on cumulative frequency distributions, because high manpower requirements cause a restriction to a limited number of samples.

Putting all these aspects together, a restraint on the discussion of the spatial distribution of annual mean SO_2-ground-level concentrations seems to be adequate to the analysis of calculated values discussed in the chapter before.

In addition to the continuous, automatic measurements cited above, the following figure 20 shows a hand analysis of random measurements for the same time period.

Bringing up some of the main criteria for the validation of calculated concentration field structures, as formulated on page 21 of this document

- positions of concentration maxima
- gradients within the concentration field
- orientation of concentration isolines,

one comes to the following conclusions

- the position of concentration maxima is reproduced quite well by measurements and by most of the models, which can easily be explained by the strong dependency of the concentration field upon population density
- the size of the concentration maxima differs by comparison between measurement and model calculation in the same order as the deviations between the models among each other (last chapter)

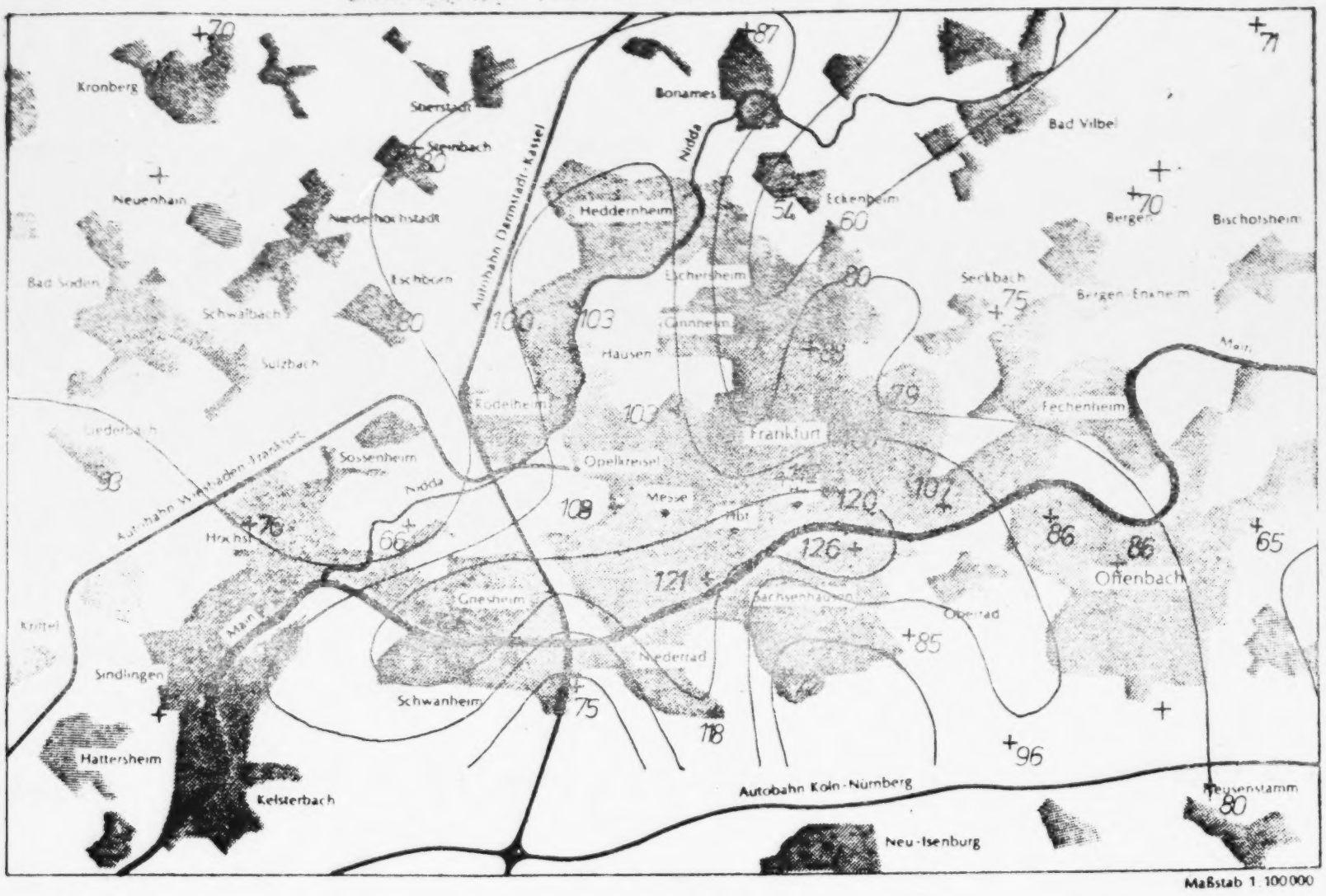

Figure 20 Random SO_2-measurement in Frankfurt area

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- the orientation of concentration isolines into the direction of the two main wind direction is found as well in the measurements as in most of the more complicated models
- nearly all models show a city-center to suburb gradient being too large, when compared with measurements, the degree of which depends on the respective emission fields in the surrounding. Possible causes have already been discussed by GUTSCHE and LENSCHOW (1973). A practicable concept to solve this problem could be leased upon GIFFORD and HANNA's concept using assumptious concerning background concentrations.

Comprehending these results it has to be emphasized that due to this comparison of several model results with available measurements

- first hints could be found concerning the capabilities and the limits of applicability of Gaussian plume models and,
- some hints are found concerning the error band width for the annual mean SO_2-ground-level concentrations combining the results of this chapter with those of the last one.

On the other hand - and that is the point where the importance of sensitivity analyses has to be manifested -, it has to be confessed that there are still several phenomena which cannot be explained or can only with difficulties, as well in the calculated as in the measured concentration fields. And there is the crux, to assess comparative model calculations in the sense of model validation the modeler would need, too, the results of a "Practical Demonstration of Urban Air Quality Measurements".

8. Summary and Conclusions

The "Practical Demonstration of Urban Air Quality Simulation Models", being the first practical model comparison broadly planned on an international basis, was an important step to realize Recommendation XIV of the NATO/CCMS Pilot Study Air Pollution (see page 2 of this document).

- It was the first attempt to bring together within the scope of a concrete, limited trial in praxis as well model developers as air quality managers for the exchange of ideas, the discussion of user's needs, and the practical demonstration of modeling techniques.

- Though there have been several difficulties to prepare a "Common Date Base" satisfying the requirements and necessities of all participating models and though there had to be made first experiences in the organisation of such a nearly world-wide model comparison, one point has to be stated: as well the methodical foundations for country-specific standardization of GAUSSian Plume-Models (see Chapter 6) could be developed as first hints for the error band widths of certain air pollution criteria to be expected from different model calculations could be derived (see Chapter 6 and 7).

- Therefore in the sense of Recommendation XIV, a continuation to review on-going air quality assessment studies on the basis of these results has to be asked for.

Summary of the Experiences made from this "Practical Demonstration of Urban Air Quality Simulation Models"

To accomplish a "Practical Demonstration of Urban Air Quality Simulation Models (GAUSSian Plume)" the outer boundary conditions, for example:

- form (e.g. annual mean concentrations or higher percentils)
- structure (e. g. point values at receptor sites or areal mean values)
- and interpretation

of the model output, have to be set by an Air Quality Management System, taking into account health criteria, socio-economic and political necessities, environmental and ecological efforts, and availability of adequate data sets.

Bearing this in mind, the internal criteria for preparing a data base for this "Practical Demonstration" have to be derived from these in a so-called PQRSTUV-sequence:

P - Postulates of the AQMS

Q - Quality and completeness of input data considering necessities and requirements of all participating models

R - Representativity and uniform description of input and output data (model results)

S - Sensitivity analyses of data uncertainties and model as well as parameter assumptions

T - Transferability of modeling methods and interpretation statements

U - Universality within the scope of the applicability (see Chapter 2) of a GAUSSian plume model

V - experimental Verification and Validation of the model

All these different aspects have to be seen as a fundamental entirety. Prescribed criteria concerning evaluation as well as assessment methods for the model output, the choice of the respective model type, quality and extent of model input data, and model validation procedures can be derived in a quite straightforward way. The consequence is, that due to the differentiated requirements of several Air Quality Management Systems not just "one perfect model" seems to be adequate to answer all essential air pollution problems; this can only be expected by a problem-specific differentiated module system of different, but individual models, being compatible between one another, as an integral concept for air quality management.

9. Literature

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Appendix I: List of Participants in the Practical Demonstration of Urban Air Quality Simulation Models

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Appendix II: Continuously Measured Concentration Data for Selected Receptor Sites

Coordinates of receptor sites, for which continuous, automatic measurements are available

Receptor-Site	GAUSS-KRÜGER Coord.	"Test-City"-Coord.
Zentralstation	347570; 555410	2470; 2910
Niedererlenbach	347890; 556220	2790; 3720
Nied	347010; 555250	1910; 2750
Offenbach	348100; 555260	3000; 2760
Hattersheim	346220; 554710	1120; 2210
Neu-Isenburg	347920; 554750	2820; 2250
Großkrotzenburg	349670; 555040	4570; 2540

ANNEX I

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ANNEX II

NATO/CCMS Documents on the First Air Pollution Pilot Study (available at: NATO/Committee on the Challenges of Modern Society, NATO Headquarters, Brussels, Belgium)

AIR POLLUTION (No. 5)

Proceedings of the 2nd Meeting of the Expert Panel on Air Pollution Modeling, (26 - 27 July 1971, Paris, France). Out of stock

AIR POLLUTION (No. 6)

Guidelines to Assessment of Air Quality (Revised)

APPENDIX A	Assessment of Air Quality in Ankara (February 1973)
APPENDIX B	Assessment of Air Quality in St. Louis (February 1973)
APPENDIX C	Assessment of Air Quality in Frankfurt (June 1974)
APPENDIX D	Assessment of Air Quality in Oslo (February 1973)
APPENDIX E	Assessment of Air Quality in the South Holland Region (December 1973)

AIR POLLUTION (No. 7)

Quality Criteria for Sulphur Oxides (November 1971). Out of stock

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Air Quality Criteria for Carbon Monoxide (June 1972)

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Control Techniques for Sulphur Oxide Air Pollutants (October 1973)

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AIR POLLUTION (No. 41)

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AIR POLLUTION (No. 50)

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ANNEX III

NATO/CCMS Documents on the Pilot Study on Air Pollution Assessment Methodology and Modeling
(available at: NATO/Committee on the Challenges of Modern Society, NATO Headquarters, Brussels, Belgium)

Air Pollution (No. 42)

Proceedings of the 6th International Technical Meeting on Air Pollution Modeling and its Application
(24 - 26 September 1976, Frankfurt/Main, Germany)

Air Pollution (No. 51)

Proceedings of the 7th International Technical Meeting on Air Pollution Modeling and its Application
(7 - 10 September 1976, Airlie House, USA)

Air Pollution (No. 70)

Bibliography on Grey Literature on Air Quality Modeling, Part I (Applied Models) (October 1977)

Air Pollution (No. 71)

Air Quality Management Systems (AQMS) (October 1977)

Air Pollution (No. 88)

Bibliography on Grey Literature on Air Quality Modeling, Part II (New Modeling Techniques) (October 1978)

Air Pollution (No. 89)

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Air Pollution (No. 80)

Proceedings of the 8th International Technical Meeting on Air Pollution Modeling and its Application
(20 - 23 September 1977, Louvain-la-Neuve, Belgium)

Air Pollution (No. 99)

Introduction to Air Quality Modeling (October 1978)

Air Pollution (No. 100)

Air Pollution Emissions Projecting (October 1978)

Air Pollution (No. 101)

Uses and Needs for Air Quality Modeling (May 1979)

Air Pollution (No. 102)

Fundamentals for the Application of a Gaussian Plume Model (April 1979)

Air Pollution (No. 104)

Air Pollution Emissions Inventory Systems
(October 1978/July 1979)

APPENDIX A: Emissions Inventory in Belgium
APPENDIX B: Emissions Inventory in Canada
APPENDIX C: Emissions Inventory in Germany, Federal Republic of
APPENDIX D: Emissions Inventory in The Netherlands
APPENDIX E: Emissions Inventory in Norway
APPENDIX F: Emissions Inventory in the United States of America

Air Pollution (No. 106)

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Air Pollution (No. 105)

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Air Pollution (No. 103)

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Proceedings of the 10th International Technical Meeting on Air Pollution Modeling and its Application
(23 - 26 October, 1979, Roma, Italy)